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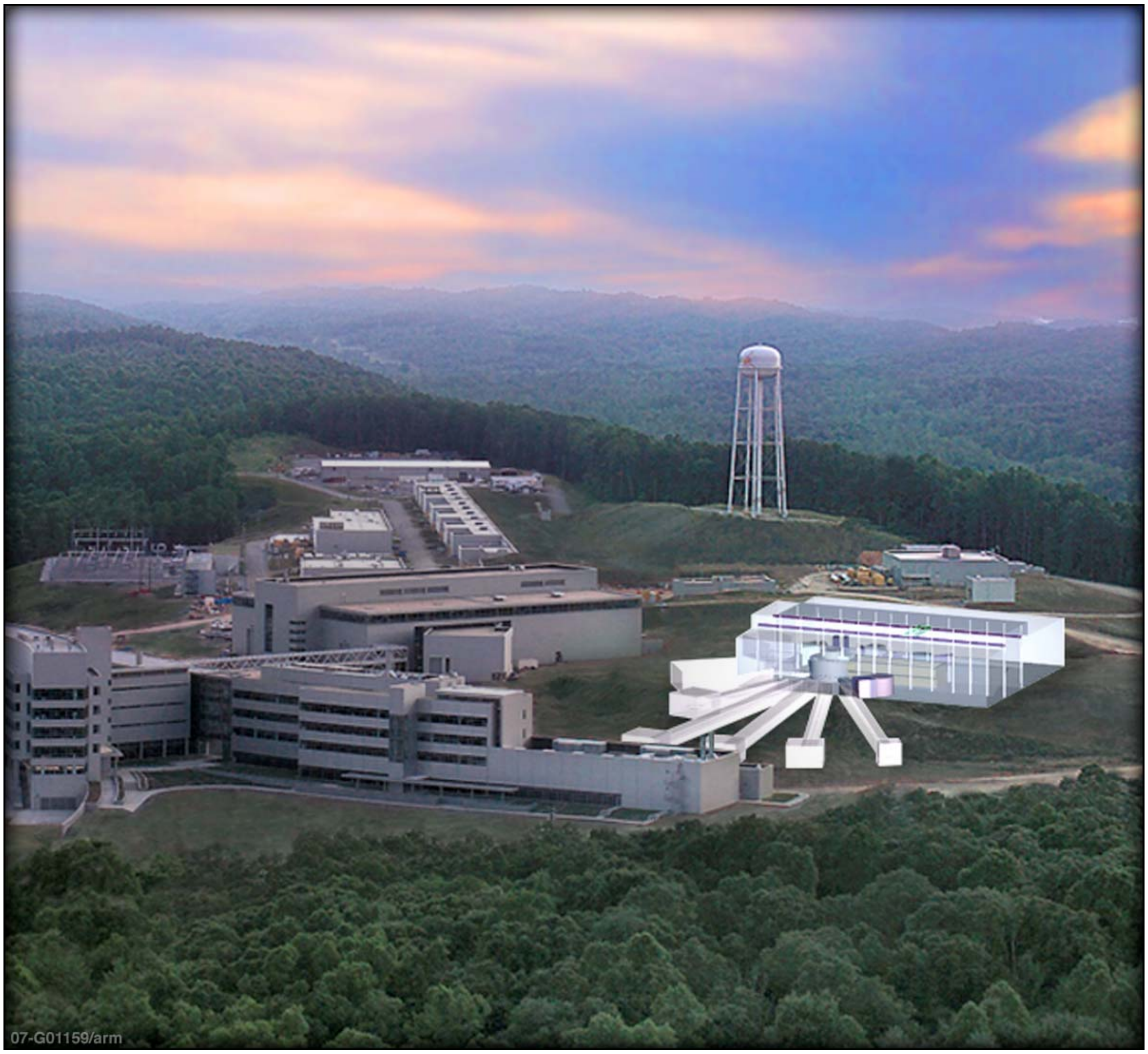
CONCEPTUAL DESIGN STUDY FOR A SECOND TARGET STATION FOR THE SPALLATION NEUTRON SOURCE



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SNS Second Target Station

Conceptual Design Study

September 2008

Based on an internal document produced by the SNS Second Target Station Working Group in October 2007

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ABBREVIATIONS, ACRONYMS, AND INITIALISMS

AB	amine borane
AECM	architect-engineer construction manager
ANL	Argonne National Laboratory
BESAC	Basic Energy Sciences Advisory Committee
CCL	coupled-cavity linac
CD-0	Critical Decision 0, DOE approval of mission need
CEF	Central Exhaust Facility
CLO	Central Lab and Office building
CMMP	condensed matter and materials physics
CMMS	condensed matter and materials sciences
CNCS	Cold Neutron Chopper Spectrometer
CUB	Central Utilities Building
DOE	Department of Energy
EQSANS	Extended Q-Range SANS (instrument at FTS)
ESS	European Spallation Source
FOM	figure of merit
FTS	SNS first target station
FWHM	full width at half maximum
GID	grazing-incidence diffraction
GISANS	grazing-incidence SANS
GMR	giant magnetoresistance
GPa	giga-Pascal
HEBT	High Energy Beam Transport
HFIR	High Flux Isotope Reactor (at ORNL)
HiMaNDi	high-throughput MaNDi
HMI	Hahn-Meitner Institute (reactor-based neutron scattering facility in Germany
HVCM	High Voltage Converter Modulator
ILL	Institut Laue Langevin (reactor-based neutron scattering facility in France)
IRP	inner reflector plug
ISIS	pulsed spallation neutron source in the United Kingdom
J-PARC	Japanese intense pulsed neutron source facility
LWTS	Long Wavelength Target Station
MaNDi	macromolecular neutron diffractometer
MAPS	a neutron chopper spectrometer at ISIS
MBE	molecular beam epitaxy
MIEZE	modulation of intensity with zero effort
MOKE	magneto-optic Kerr effect
nEDM	experiment to measure the electric dipole moment of the neutron
NRSE	neutron resonance spin-echo
NSE	neutron spin-echo

NSF	National Science Foundation
ORNL	Oak Ridge National Laboratory
PUP	Power Upgrade Project (at SNS)
R&D	research and development
RF	radio frequency
RFQ	radio-frequency quadrupole
RRM	repetition rate multiplication
RTBT	Ring to Target Beam Transport
SANS	small angle neutron scattering
SCL	superconducting linac
SERGIS	spin-echo-resolved grazing incidence scattering
SESANS	spin-echo small angle neutron scattering
SING-II	SNS Instruments Next Generation II, project to build 5 neutron-scattering instruments at FTS
SNS	Spallation Neutron Source (at ORNL)
STS	SNS second target station
T_c	transition temperature
TISANE	time-resolved small angle neutron experiments
TOF	time-of-flight
TSB	target service bay
UCN	ultra-cold neutron
VCNS	very cold neutron source
WBS	work breakdown structure

PREFACE

This document is a slightly abbreviated version based on the internal White Paper prepared by the SNS Second Target Station Working Group in October 2007. Most of the text in this present document was taken directly from that White Paper, but the opportunity has been taken to correct minor typographical errors and to add clarification in a few places. Since the original White Paper was produced, the acronyms for the first and second target stations at SNS were changed to FTS and STS respectively. Those changes have been introduced throughout the present document.

The SNS Second Target Station Working Group members were H. Bilheux, R. K. Crawford, R. Dean, P. Ferguson, J. Galambos, K. Herwig, T. McManamy, H. Mook, R. Pynn, G. Smith, and A. Stoica, with significant additional input by F. Gallmeier and M. Rennich. However, the White Paper represents the work of many others as well and is the culmination of a process that began with a scoping workshop in August, 2006, followed by two more workshops and numerous internal studies and analyses.

A large number of other people both from within ORNL and from external national and international institutions contributed to the process leading to that White paper and subsequently to this document, which would have been impossible without the considerable amount of input they provided. Furthermore, the three very useful workshops that were part of this process would not have been possible without significant assistance from a number of administrative staff within the Neutron Sciences Directorate and within other support organizations at ORNL. And finally, thanks go to the Communications staff, and especially to Deborah Counce, for the editing of the White Paper from which this document derives its content.

EXECUTIVE SUMMARY

In keeping with the BES 20-year plan, the Oak Ridge National Laboratory (ORNL) Neutron Sciences Directorate has conducted a study during 2006-2007 to understand the new scientific capabilities that could be offered by the various options for a second target station at the SNS. As part of this study, one set of options was selected as a reference concept to be evaluated in detail. This concept is optimized for the production of intense beams of cold neutrons. In this reference concept the SNS accelerator system is operated in a "pulse-stealing" mode at 60 Hz with every third pulse going to the second target station (20 Hz second target station operation) and the remainder of the pulses going to the first (present) SNS target station (40 pulses per second in a "pseudo-60 Hz mode"). For the 20 pulses per second going to the second target station, the long proton pulse (~1 ms long) from the linac is sent directly to the second target station with no accumulation in the ring, thus giving 50% more power to the second target station with no increase in peak linac current. This concept employs a mercury target that is low-risk because the long proton pulse significantly diminishes any mercury cavitation effects. The baseline case is 1.33 MW to the first target and 1 MW to the second target, with potential for eventual operation at 2 MW and 1.5 MW respectively.

The detailed evaluation of this reference concept showed that **a second target station for the SNS could provide more than an order of magnitude improvement in performance for broad areas of forefront science, thereby opening up totally new areas to exploration with the full power of neutron scattering techniques.** In particular, **for the first time neutron scattering will be extended to span the full dynamical range from picoseconds to minutes,** by utilizing the high intensity of cold neutrons at the proposed second target station to extend neutron-spin-echo studies of slow motions by an order of magnitude to longer times (up to 10 microseconds) and to use sample modulation techniques to extend kinetic studies down to times as short as 10 microseconds. The intense cold neutron beams will also permit tightening the angular resolution to provide an order-of-magnitude extension of neutron scattering dynamical studies to probe such slow motions over longer length scales (up to 1 micron) , and will enable **the use of focused 10 micron neutron beams** to study extremely small samples and to provide totally new neutron imaging capabilities. In addition, these high intensities of cold neutrons will provide revolutionary new capabilities to probe **lateral structures on surfaces and membranes at length scales from 10 to 1000 nanometers**.

Hence the quantum jump in performance brought by the second target station will provide researchers with the means to probe distance and time scales that have hitherto been unavailable, but are critical to answering some of the grand challenge questions facing our society. Extending the range of measurement to longer distances and slower time scales enables the study of systems exhibiting **greater complexity**, such as the complex chemical systems that occur in many soft matter studies, aspects of macromolecular functionality important in biology that can be explored using neutron scattering, or the multi-component systems important to the geophysical properties and functions relevant to earth sciences. Furthermore the unprecendented high intensities will also enable very short measurement times with the routine use of parametric studies to explore **systems far from equilibrium, in transient states, or in approach to equilibrium**.

In addition to these unique capabilities, the high intensities of cold neutrons will enable smaller samples to be measured, under more complex environments, thereby providing information on materials under extreme conditions hitherto unattainable.

The optimization chosen for the reference concept for the second target station focused on producing the most intense cold neutron beams, complementary to the present SNS target station focus on the production of short neutron pulses for high-resolution studies with epithermal, thermal, and cold neutrons. This difference in focus of the optimization of the two target stations makes them highly complementary, and allows the second target station to provide cold beam intensities much higher than those available at the first target station.

This second target station facility would provide the US research community with a powerful and unique suite of measurement tools comparable in scope to those provided by the present SNS, roughly doubling the number of users that could be accommodated and offering the capability to address critical challenges by extending the capabilities of neutron scattering techniques to realms that have heretofore been inaccessible.

SNS Second Target Station

1.0 OVERVIEW

1.1 BACKGROUND

The Spallation Neutron Source (SNS) facility at Oak Ridge National Laboratory (ORNL) became operational in the spring of 2006. The basis recommendations for the SNS facility were articulated in a report to the Department of Energy (DOE) in February 1996 by a committee chaired by Dr. Thomas Russell. This report specified that the SNS should be a pulsed spallation neutron source capable of 1 MW operation and dedicated to neutron scattering. It also specified that the design and implementation of the SNS should be such that the power of the facility could be upgraded with minimal disturbance, and that the facility design should include the "capability of additional targets, as required, with multiplexing to accommodate an expanding experimental instrument suite." All of these recommendations were followed in the design and construction of the SNS. Furthermore, a Basic Energy Sciences Advisory Committee (BESAC) report to DOE in 2003 led to the establishment of a 20-year plan for major DOE construction projects for Basic Energy Sciences. This 20-year plan included as high priorities both a power upgrade for SNS and a second target station for SNS. The SNS Power Upgrade Project (PUP) has already received CD-0 approval from DOE. The BESAC report strongly endorsed the second target station project as well, and "recommends planning for CD-0 before 2010." (CD-0 is DOE approval of the Mission Need for this project.)

In 2000, the National Science Foundation (NSF) commissioned a study to develop a technical design concept and the scientific case for a second target station at SNS. This study was originally intended to lead to a full proposal for funding for the second target station facility, but for various reasons the process was terminated before that proposal was submitted. Nevertheless, the results of the study were published as a joint Argonne National Laboratory (ANL) and SNS technical report [1.1]. That study was based on the assumption of 60 Hz, 2 MW, short-pulse operation of the SNS accelerator systems, with the second target station taking one of every six proton pulses and the other five pulses going to the first target station. This study showed that under these conditions, a second target station, referred to in the study as the Long Wavelength Target Station (LWTS), could be optimized to provide performance gains of a factor of 3 or more relative to the first target station for many types of scientific studies. The LWTS would, of course, have had the added advantage of roughly doubling the number of neutron scattering instruments that could be operating simultaneously at the SNS.

Within the same time frame, there was a major activity in Europe to develop the scientific case and technical concepts for the proposed European Spallation Source (ESS). The ESS was proposed to have two target stations and associated instrument suites, one 5 MW short-pulse and one 5 MW long-pulse, and extensive scientific cases and optimized suites of instruments were developed for each. Unfortunately, it proved impossible for the countries involved to arrange the funding for this ambitious project given the economic climate and other pressing priorities at that time. The full technical and scientific cases for this version of the ESS were well documented [1.2, 1.3], and subsequent work relating to a potential future ESS has been proceeding at a substantially lower level of effort.

Also within this time frame, the Rutherford-Appleton Laboratory in the United Kingdom developed and constructed a second target station at the very successful ISIS spallation neutron source facility, with the first neutron production from the second target station scheduled for the fall of 2007. *[Note added: First neutrons were measured at the ISIS second target station in August, 2008.]* An extensive science case was also prepared in support of this second target station project [1.4]. This new facility will operate in the pulse-stealing mode, with one proton pulse in five going to the second target station and the other four going to the first target station. Total beam power at the second target station will reach nearly 50 kW when it is fully operational. The target-moderator-reflector system in this second target station has been optimized to provide the best performance for a specific suite of instruments, which were in turn selected based on the scientific case developed.

With the completion of the construction of the SNS facility at ORNL, it is now time to begin planning for a project to design and construct a second target station at that facility. The urgency for the SNS second target station planning is heightened by the fact that the 24 beamlines at the first target station are already more than 80% subscribed with approved and funded instruments, and by the fact that an optimized SNS second target station is likely to benefit from significant pre-conceptual research and development and optimization studies prior to development of a full conceptual design. Planning for such a facility can draw heavily from the recent studies cited above. However, conditions have changed since the earlier LWTS study (e.g., higher SNS accelerator power will be available because of the PUP, and many instruments are already operational or are being built at the first target station), so the current planning has not been constrained to employ the same target facility concepts developed in that earlier study.

Accordingly, in order to evaluate the scientific potential of a second target station facility at the SNS, the Neutron Sciences Directorate at ORNL has been engaged in a process to define what new scientific capabilities could be made available if such a second target station were to be built. The bulk of this white paper outlines this process and presents the results obtained.

The reason for building any new research facility is the new scientific capabilities and opportunities it provides. Chapter 2 provides a look at the types of scientific opportunities that could be provided by a second target station at the SNS. It provides the guidance for focusing the second target station efforts where the greatest scientific impacts should be possible. Subsequent chapters develop the facility concepts that flow from this guidance and evaluate the performance to be expected from such a facility.

1.2 SUMMARY

1.2.1 Reference Concept

As part of this study, one set of options was selected as a reference concept to be evaluated in detail. This reference concept is optimized for the production of intense beams of cold neutrons, thus emphasizing areas of science for which the first target station was not fully optimized. In this reference concept the accelerator system operates in a “pulse-stealing” mode at 60 Hz with every third pulse going to the second target station (20 Hz second target station operation) and the remainder of the pulses going to the first (present) SNS target station (40 pulses per second in a “pseudo-60 Hz mode”). For the 20 pulses per second going to the second target station, the long proton pulse (~1 ms long) from the linac is sent directly to the second target station with no accumulation in the ring. This “long-pulse” operating mode enables the delivery of more power to the second target station for the same pulse duration, because the chopping of the proton beam necessary for storage and extraction in the ring can be eliminated. The use of long proton pulses also allows the use of a mercury target for the reference concept for the second target station even at the higher power per pulse, because spreading the proton pulse out over ~1 ms significantly diminishes any mercury cavitation effects. This white paper provides the reasoning behind these choices for the reference concept.

The detailed evaluation of the reference concept showed that **a second target station for the SNS could provide more than an order of magnitude improvement in performance for broad areas of forefront science, with the potential of opening up totally new areas to exploration with the full power of neutron scattering techniques.** It further showed that such a second target station would have low technical risk. The new capabilities provided by this second target station will position the United States to remain in the forefront of neutron scattering and the important scientific areas it can address for a number of decades into the future.

1.2.2 New Scientific Capabilities

The overarching principle guiding the choices made for the Second Target Station reference concept was **scientific optimization**. The reason for building any new research facility is the new scientific capabilities and opportunities it will provide. When considering a potential facility that by necessity will not come on line until many years in the future, it is impossible to predict the specific scientific problems this facility will be called on to address. However, several recent surveys (summarized in Chapter 2 of this white paper) of the fields currently and potentially addressed by neutron scattering show **three major themes** appearing throughout the discussions of forefront science. The first is the desire to extend current capabilities to be able to **answer more difficult questions**. These may involve extending measurements to higher resolution, performing the measurements in the presence of a more difficult sample environment and concomitant restrictions to smaller samples, or measurements made to higher precision to look for subtle intensity variations or line shape effects. The second is the desire to extend most types of measurements to **parametric studies** exploring ranges of compositions, external fields such as temperature or pressure, or time scales, as in kinetic studies. The third is the general tendency toward the study of systems exhibiting **greater complexity**, such as the complex chemical systems that occur in many soft matter studies, aspects of macromolecular functionality important in biology that can be explored using neutron scattering, or the multi-component systems important to the geophysical properties and functions relevant to earth sciences. These trends are all evident today as scientists stretch the capabilities of existing neutron sources and instrumentation to try to extend their measurements into some of these areas. It seems almost certain that regardless of which specific scientific problems move to the forefront in the future, these themes of greater difficulty, greater complexity, and parametric studies will continue in their prominence; therefore, these themes have been given primary consideration in the selection of the most promising options for the SNS second target station.

This white paper demonstrates that the SNS Second Target Station will provide major new capabilities that support these three themes and significantly extend the types of scientific problems that can be fruitfully addressed with neutron scattering. By focusing on and optimizing for the production of cold neutrons this new facility will provide much higher cold-neutron intensities than heretofore available on any pulsed neutron source. The evaluation of the performance of the reference suite of instruments with the reference accelerator and target station concept indicated that on the average these **instruments at the second target station would have data rates at least an order of magnitude better at the second target station than would similarly optimized instruments at the first target station**. These higher data rates translate into the ability to study much smaller samples, more-weakly-scattering processes, and/or higher-rate kinetic behaviors. They also translate into the ability to extend measurements to study larger length scales and slower dynamical processes. This quantum jump in performance brought by the second target station will lead to qualitatively new scientific capabilities, complementary to those at the first SNS target station. **This new facility would add a new suite of scientific capabilities comparable in scope to those provided by the present SNS, including its power upgrade project, roughly doubling the number of users that could be accommodated and providing extremely exciting opportunities to extend the power of neutron scattering into scientific areas and specific types of problems that have heretofore been inaccessible.**

As one example, these higher intensities permit tightening the resolution to provide an order-of-magnitude extension of neutron scattering dynamical studies to probe longer time scales (slower motions) at longer length scales (times up to 10 microseconds at distances up to 1 micron). This order-of-magnitude range extension will lead directly to new insights into forefront highly complex and difficult problems. One example is the “Grand Challenge” question: ‘What are the detailed processes and molecular drivers leading to the folding of proteins that is essential for them to carry out their biological role’.

Another example of new science that will be enabled with the second target station can be found in the field of neutron reflectometry, which has long been a unique and powerful tool for probing the atomic or magnetic density normal to surfaces and layered materials. In principle, lateral structures in such systems can also be probed on neutron reflectometers, using grazing-incidence techniques such as grazing-incidence diffraction or grazing-incidence SANS. However, the extremely weak signals have made the use of such techniques very difficult, if not impossible, with the neutron beam intensities that have been available up to now. The much higher intensity of cold neutrons provided by the second target station, coupled with emerging new techniques such as spin-echo resolved grazing-incidence scattering, will enable the full capabilities of neutrons (isotopic sensitivity, magnetic moment) to be brought to bear in the study of such lateral surface structures at length scales of about 10 nanometers to 1000 nanometers or more. This exciting prospect will open up broad forefront scientific areas to study with neutrons, including lateral structures in lubricating or adhesive layers, wetting phenomena, block copolymer or liquid crystal layers on surfaces, artificial biomembranes or biomimetic systems, self-assembly of nanoparticles on surface templates, and perhaps even real biological membranes.

A third example of new capabilities lies in the use of very highly focused neutron beams. At present, neutron focusing devices easily achieve focused beam sizes of < 100 microns, and focused neutron beams ~10 microns in size will be possible in the near future. The neutron intensity that will be available in such focused beams at the second target station will be enough to measure the very weak absorption or scattering produced by the relatively small number of sample atoms illuminated by a beam of this size. This, of course, will permit the study of such very small samples, and should also create opportunities to develop instrumentation for various types of scanning neutron probes for exploring minute regions of larger samples. The availability of intense neutron beams of this size will generate new techniques that will open up totally new scientific fields with an ultimate potential that is at present only dimly imagined.

As a final example of new scientific capabilities provided by the second target station, we mention the area of kinetic studies. The high flux of cold neutrons will allow all structural and dynamical measurements to be made much faster. This will, of course, facilitate parametric measurements probing material structures and dynamics as functions of environmental conditions such as temperature, pressure, applied magnetic or electrical field, or changing chemical composition of the environment. However, perhaps even more exciting, these rapid measurements will allow structural measurements (at length scales ranging from hundreds of nanometers down to fractions of one nanometer) to be made in a few seconds or less, allowing the kinetics of relaxation processes or the approach to chemical equilibrium to be followed on such time scales. This will enable much more extensive neutron exploration of the behavior of systems far from equilibrium and the approach to equilibrium than has previously been possible. In favorable cases pump-probe or other sample modulation techniques can extend these types of measurements down to a few microseconds, allowing much more detailed study of the initial relaxations in far-from-equilibrium conditions in a wide variety of systems. Thus the second target station will enable neutron scattering to make major contributions to this Grand Challenge area as well.

1.2.3 Complementary to the Present SNS Target Station and to HFIR

The first target station at SNS was optimized primarily to produce short neutron pulses for high-resolution studies with epithermal, thermal, and cold neutrons. Therefore, the cold neutron beams at the first target station are not nearly as intense as they would be in a source optimized solely for the production of cold neutrons. However, the fact that the first target station is already designed to provide the short-pulse thermal and cold beams means that the optimization of the second target station can concentrate on providing the maximum intensity of cold neutrons, with pulse length only a secondary consideration. This difference in focus of the optimization of the two target stations makes them highly complementary, and allows the second target station to provide cold beam intensities much higher than those available at the first target station. Furthermore, although there are also cold neutron beams available at HFIR, most of the scientific applications and associated instrumentation identified for the second target station in this study need to be located at a pulsed source to obtain optimal results.

1.2.4 Low Technical Risk

The final principle guiding the choices made for the reference concept is that they should have **low technical risk**, so there would be a strong assurance that a second target station facility would deliver performance at least as good as that predicted for the reference concept. Having focused on the production of cold neutrons, this study evaluated potential target-moderator-reflector configurations to find the configuration producing the best cold neutron beam performance with relatively low technical risk. The different possibilities for the proton beam pulsing rate and pulse duration to the second target station were evaluated in terms of effects on the source and instrument performance, the technical risk, and the cost and schedule impacts. In order to assess the performance in scientific terms, a reference suite of neutron beam instruments well suited to the second target station performance was defined and their performance evaluated. Very preliminary concepts for the target station and the site layout were also developed, again with a strong emphasis on the use of currently-understood technology in order to minimize technical risk. This white paper documents all of these steps that together make up the reference concept for the second target station facility at SNS.

1.2.5 Opportunities for Improvements to the Reference Concept

As noted above, the choices made for the reference concept were based on high performance with low technical risk. However, during the course of the study, a number of other options were identified that were deemed to have somewhat higher technical risk but that warranted further study because of significant potential for even higher performance, improved reliability, or lower costs. **A program of research and development and concept optimization is proposed to investigate the most promising of these options because the payoffs in performance, reliability, and/or cost might be significant if the technical risks could be mitigated.** The study also identified potential significant opportunities for **cost savings and other efficiencies that could result from a careful integration of the plans for the second target station into other activities at the SNS site**. Such other activities include the SNS power upgrade project, the choices of new instruments to be built at the SNS first target station and at HFIR, and the infrastructure upgrades necessary to support all the other new construction and new activities planned for the SNS site.

1.3 REFERENCES

1.1 J. M. Carpenter and T. E. Mason, *Technical Concepts for a Long Wavelength Target Station for the Spallation Neutron Source,* ANL-02/16, ORNL/SNS-TM-2001/163, November 2002.

1.2 The ESS Project: Vol. I, *European Source of Science*; Vol. II, *New Science and Technology for the 21st Century;* Vol. III, *Technical Report*; Vol. IV, *Instruments and User Support*. Available at http://neutron.neutron-eu.net/n_documentation/n_reports/n_ess_reports_and_more/102.

1.3 F. Mezei and R. Eccleston, *Performance of a Suite of Generic Instruments on ESS*, ESS/INST/P1/01, 2001.

1.4 Documentation for the ISIS Second Target Station Project, http://ts-2.isis.rl.ac.uk/.

2.0 SCIENCE DRIVERS FOR A SECOND TARGET STATION AT SNS

2.1 REVIEW OF PREVIOUS STUDIES

The three recent studies cited in Chapter 1 have identified areas in which more intense pulsed neutron sources coupled with current state-of-the-art instrumentation capabilities (or extensions of such capabilities) can make significant contributions to some of the fundamental scientific and technological problems currently facing our society [2.1–2.3]. Each of these studies involved workshops to assess the future role of neutron scattering across the broad range of scientific fields that can collectively be called condensed matter and materials sciences (CMMS). These workshops gathered internationally recognized experts in the respective areas to explore potential neutron contributions to the fields of solid state physics, materials science and engineering, biology and biotechnology, soft condensed matter, chemistry, earth sciences and environmental sciences, and liquids and glasses. Although not part of CMMS, these workshops also addressed the role of thermal and cold neutron beams in fundamental neutron physics studies. The topical areas covered by the three different sets of workshops are similar, and the assessments made in the workshops are consistent with one another. These assessments are still relevant, so rather than repeat the work already done with a similar series of workshops likely to draw similar conclusions, this document summarizes the highlights from all these previous workshops in Sections 2.1.1 through 2.1.8, along with a few more recent examples to illustrate some of the points. Several related studies are described briefly in Section 2.2. Section 2.3 discusses the implications of Sections 2.1.1 through 2.1.8 and those in Section 2.2 in the context of planning for a second target station at the SNS. Most of these workshops also indicated what instrumentation they thought would be needed to carry out the scientific programs envisaged. This suggested instrumentation is summarized and discussed in Section 2.3.

2.1.1 Solid State Physics

2.1.1.1 Frontier Research Areas

Solid state physics has a strong overlap with materials science. However, in solid state physics, the emphasis is more on the fundamental understanding of some overarching features such as lowered dimensionality, greater complexity, lattice effects, or non-equilibrium and time-dependent phenomena, whereas materials science focuses more directly on the development and characterization of new materials aimed at providing specific functional properties. A list of frontier areas in solid state physics includes quantum dot arrays; transport and magnetic properties in 1-dimensional systems; domain walls, domains, correlations, and grain boundaries; surfaces and thin films; interplay of spin, orbital, and charge degrees of freedom; coupled excitations; strongly interacting electron systems (Fig. 2.1); flux line lattices; phase transitions, quantum critical points; frustration; disorder and interfacial roughness; proximity effects; lattice modes; confinement; fast response to external probes and fields; magnetic fluctuations and relaxations; tunneling; molecular magnets; interfaces and hybrid structures; self-organizing molecular systems; novel magnets and superconductors; and organic materials.

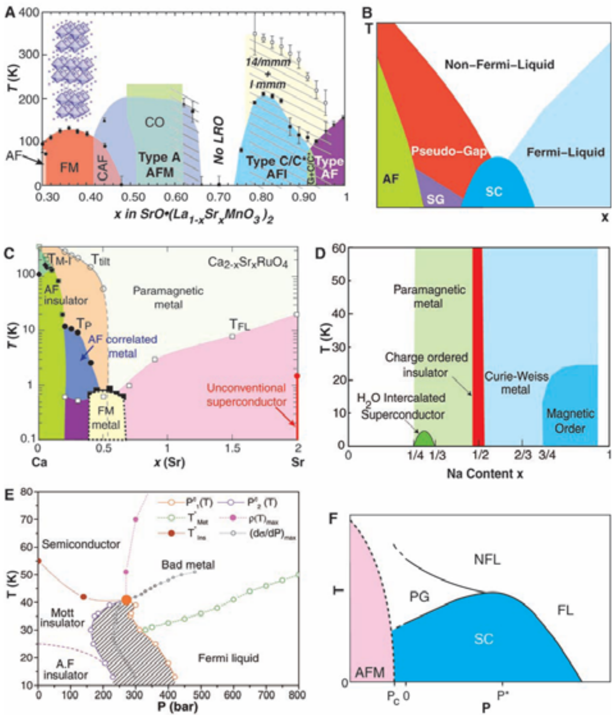

Fig. 2.1. Strongly correlated electron systems. An important characteristic of materials with strongly correlated electrons (e.g., leading to colossal magnetoresistance or high-temperature superconductivity) is the existence of several competing states, as indicated by these complicated phase diagrams of the transition metal oxides. Neutron scattering has made and will continue to make significant contributions to the understanding of strongly -correlated-electron materials. Both thermal and cold neutrons are important, but cold neutrons will be particularly important for accessing the long length scales that occur in many of the structures and dynamical processes involved. (*Source:* E. Dagotto, *Science* **309**, 5732, 257–262, 2005.)

2.1.1.2 Role of neutrons

Examples of in which where neutron scattering can play a significant role in such frontier solid state physics research are

- research in the dynamics of superlattices, thin films, wires, and dots
- lateral magnetic structures on thin films
- magnetic domain wall structure and dynamics
- quantum tunneling in molecular magnets and quantum-tunneling-induced gaps in the excitation spectra of magnetic nanoparticles
- study of spin-density distributions and waves in organic materials, molecular magnets
- revelation of exotic magnetic interactions (e.g., quadrupolar)
- lifetimes of lattice and magnetic collective modes
- physics of magnetic impurity defects at the dilute limit
- dynamical and structural studies of the effects of competing spin, charge, and lattice degrees of freedom (e.g., dynamic charge ordering in superconductors, short-range charge correlations that melt with the onset of ferromagnetism)
- spin glass dynamics

- probing of magnetic fluctuations over a wide range of energies, temperatures, and materials to address fundamental questions in quantum criticality

2.1.2 Materials Science and Engineering

2.1.2.1 Frontier research areas

Materials science and engineering have been the keys to many of the technological advances that are driving major segments of the economy today. However, the frontier areas in materials science are being extended to studies of more complex materials, in-situ and real time studies of dynamical changes and process monitoring, smaller sampling regions buried in larger components, samples in complex environments, and samples in extreme environments.

2.1.2.2 Role of neutrons

For many years neutron scattering has been an important tool for characterizing new materials and for elucidating the relationships between the structure and dynamics of the material and the functional properties of interest. Some examples of frontier areas include using structural, kinetic, or dynamical neutron scattering measurements to provide essential information for

- understanding the process of lubrication and its relationship to the properties of the lubricant and the lubricant-surface interactions
- understanding mechanisms of deformation and damage and validation of models used for engineering design and assessment
- better understanding of magnetic storage and readout devices (Fig. 2.2), including understanding the effects of spin structures and fluctuations
- process monitoring and optimization
- monitoring the hydrogen locations and motions and the optimization of processes and materials in energy storage systems and energy conversion devices

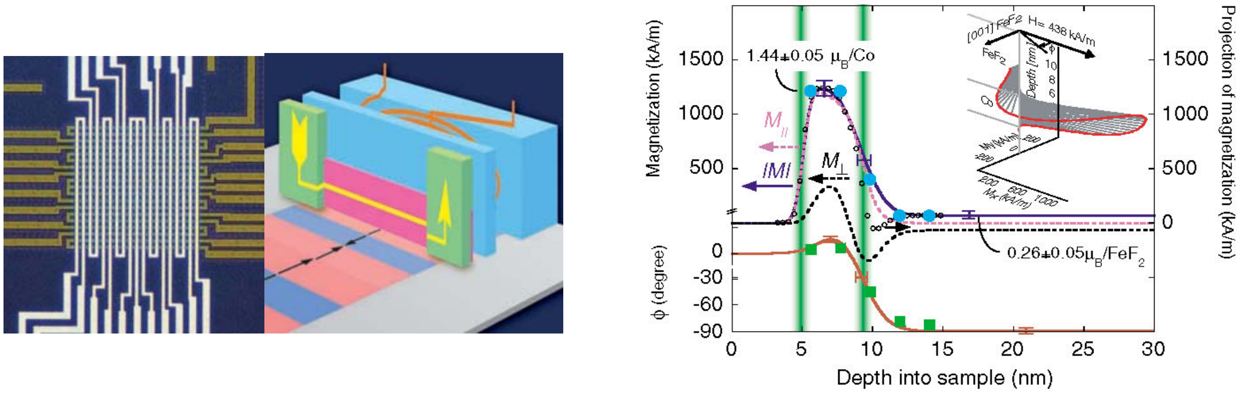

Fig. 2.2. Magnetic devices probed with neutron reflectometry. Left: a magnetic random access circuit and a spin-valve read head for a hard drive, two devices that depend on exchange bias from thin antiferromagnetic layers. Right: the depth dependence of the magnitude (blue curve) and angular deviation (red curve) obtained from polarized neutron reflectivity measurements from a similar layered magnetic structure (symbols are from simulations). (*Sources*: Left—M. Fitzsimmons and S. K. Sinha, *Los Alamos Science* **30**, 178–185, 2006; Right—S. Roy et al., *Phys. Rev. Lett.* **95**, 047201, 2005.)

2.1.3 Chemical Structure, Kinetics, and Dynamics

2.1.3.1 Frontier research areas

Some of the frontier areas in materials chemistry include smart materials that respond to their environments; thin films to build devices; hydrogen storage materials (Fig. 2.3); and the structure and dynamical characterization of very small quantities of pharmaceuticals, catalysts, or other novel materials.

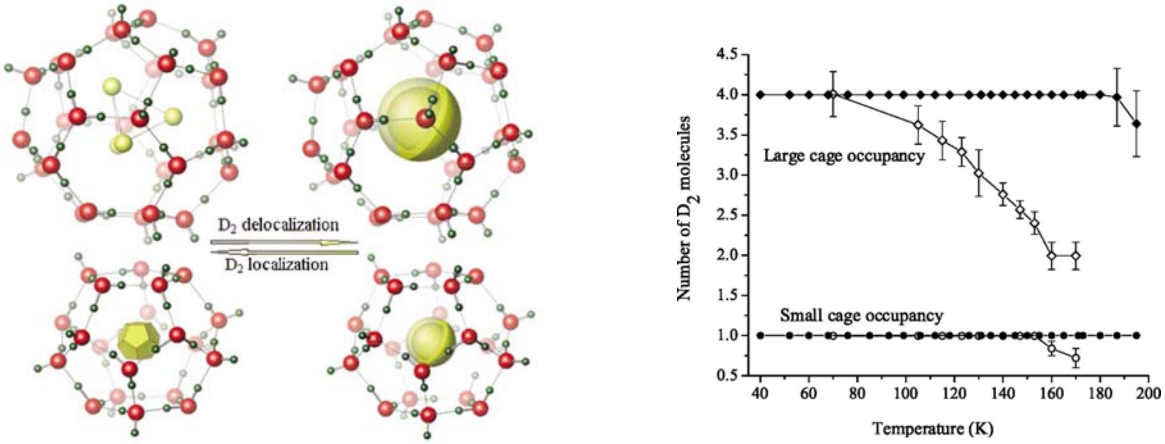

Fig. 2.3. D_2 distribution in D2–D2O clathrate, a potential hydrogen storage material. Left: locations of guest D_2 molecules are shown in the framework structure, showing delocalization that occurs above 50 K. Right: the occupation of these locations is shown as determined by neutron diffraction (open and closed symbols represent data obtained at ambient and 2 kbar pressures). Neutrons have been used to probe the kinetics of the charging process in this and similar materials. A range of distance and energy scales come into play in such systems, and portions of this range can best be probed with cold neutrons. (*Source*: K. Lokshin et al., *Phys. Rev. Lett.* **93**, 125503, 2004.)

2.1.3.2 Role of neutrons

Important areas in which neutron scattering studies are needed to provide essential information include

- energy storage and conversion materials and processes, including studies of faster processes
- in-situ studies of catalysts, including kinetic studies
- ultra-high-resolution structural studies of subtle features and distortions important to the functionality of a variety of complex crystalline structures
- structural studies over multiple length scales extending to nanometer dimensions, important for understanding mesoporous materials and self-assemblies of nanometer-scale building blocks
- hydrogen bonding and proton dynamics in advanced materials
- diffusion in porous materials
- rotational tunneling and the obtaining of precise rotational potentials
- electrochemistry at surfaces with realistic samples
- in-situ monitoring of polymer synthesis

- chemical kinetics, including cyclic electrochemical processes

2.1.4 Soft Condensed Matter

2.1.4.1 Frontier research areas

The research topic of “soft matter” includes an extensive range of molecular materials such as polymers, liquid crystals, micellar solutions, microemulsions and colloidal suspensions, and biological membranes and vesicles (Fig. 2.4). Such materials have a wide range of applications as diverse as structural and packaging materials, foams and adhesives, detergents, cosmetics, paints, food additives, lubricants and fuel additives, and rubber in tires.

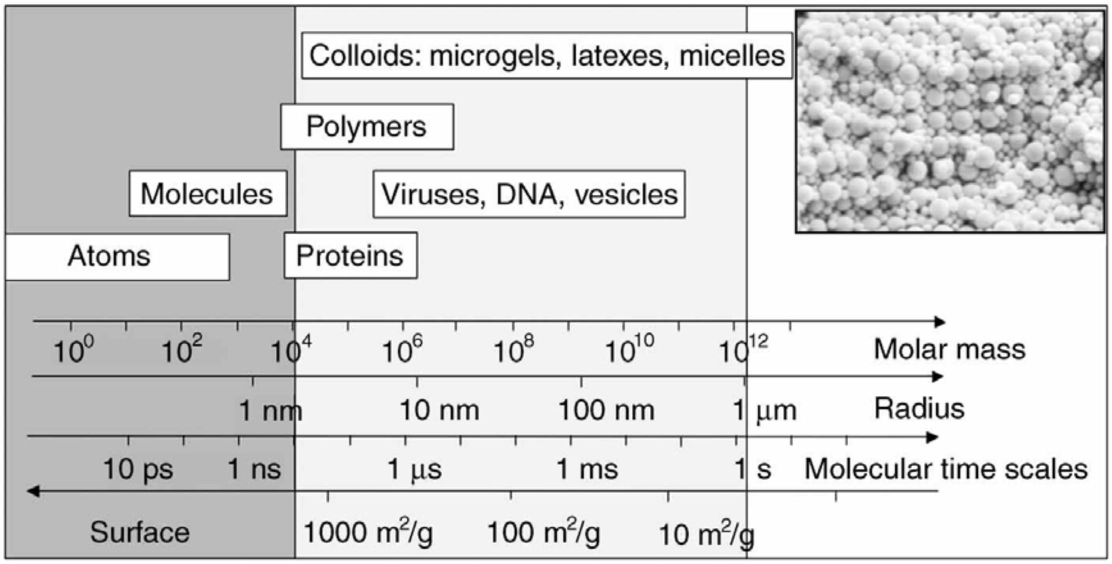

Fig. 2.4. Length and time scales relevant for soft matter systems. The inset shows a crystallized colloid. Neutrons are particularly good for obtaining both static and dynamic information from such hydrogen-containing materials; several different instruments will be needed, each optimized to use either thermal or cold neutrons as required, in order to access these full ranges. (*Source*: L. J. Magid and P. Schurtenberger, *MRS Bulletin* December, 907–912, 2003.)

2.1.4.2 Role of neutrons

Some examples of forefront areas where neutrons can play a prominent role are

- molecular rheology, important for industrial processing
- buried interfaces such as the liquid-liquid interfaces important in understanding the stability of emulsions and in biolubrication
- smaller sampling volumes to probe local regions of bilayers or biomolecular or polymeric ultrathin microelectronics and photonics films in-situ
- time-evolution structural studies of self-assembled phases, including systems containing natural or synthetic proteins and nucleic acids with lipids and polymers
- conformational transformations in biomacromolecules
- synthesis, aggregation, and transport of minerals in biology
- the role of self-assembly in plant growth

- new materials produced by external constraints such as shear
- structure, interactions, and dynamics of complex hybrid materials such as soft-hard nanocomposites and complex polymers in polymer mixtures or blends or in solution
- effects of confinement and extreme environments on phase behavior, thermodynamics, and transport properties of complex liquids, including studies of such liquids in porous materials when the sizes of the structural units in the liquids approach the pore sizes
- probing of the molecular dynamics of noncrystalline matter (most of the soft materials) and the role of intramolecular dynamics in controlling the macroscopic responses of soft-matter-based materials

2.1.5 Liquids and Glasses

2.1.5.1 Frontier research areas

Most real materials are not well-ordered crystals, so the study of disordered materials is of high importance. The goal is to understand how the structure and dynamics in such systems control the macroscopic properties. The forefront has moved beyond the study of model systems to more complex systems, and trends are expected to continue toward greater levels of complexity.

2.1.5.2 Role of neutrons

Important research areas that can be addressed with neutrons include

- fundamental studies of the atomic dynamics of disordered matter, including information on the dynamics of individual atom types in multi-component systems, determination of the shapes and widths of the inelastic (“Brillouin”) and elastic (“Rayleigh”) lines, and understanding of the two-level tunneling states
- fragility, the Boson peak, and relaxation in glassy materials
- determination of the effects of ions or other entities in solution on the solvent structure, including the effects of ions in combination, and extending to the exploration of the aqueous environments of large molecules in solution in the presence of different ions
- the role of disorder in water or water-rich solutions on hydrolysis reactions, the mobility of drugs and nutrients in organs, the mobility of nutrients in soils, proton conduction in liquid electrolytes, entrapment of water in concrete, and denaturation of proteins
- understanding of the atomic and magnetic structure of soft or hard metallic glasses with at least three atomic species
- structural measurements of multi-component ionic-conductor systems and dynamical measurements of the diffusion of dilute ionic species or the relaxation of polymers over a wide time scale
- structures of glasses in the presence of dilute impurities
- kinetics and structural aspects of phase transitions, including the liquid-glass transition, the study of phase separations in supercritical systems, and glass formation using sol-gel processes
- impacts of disorder, doping, or confinement on Bose-Einstein condensation superconductivity; phase transitions; and magnetic, thermodynamic, elastic, chemical, and biological properties

- migration of liquids in porous media and ion migration in glasses.

2.1.6 Biology and Biotechnology

2.1.6.1 Frontier research areas

The forefront activities of life sciences at the molecular and cellular scale (Fig. 2.5) are functional genomics and proteomics. It will be important to obtain specific functional information on most proteins encoded in the human and other genomes.

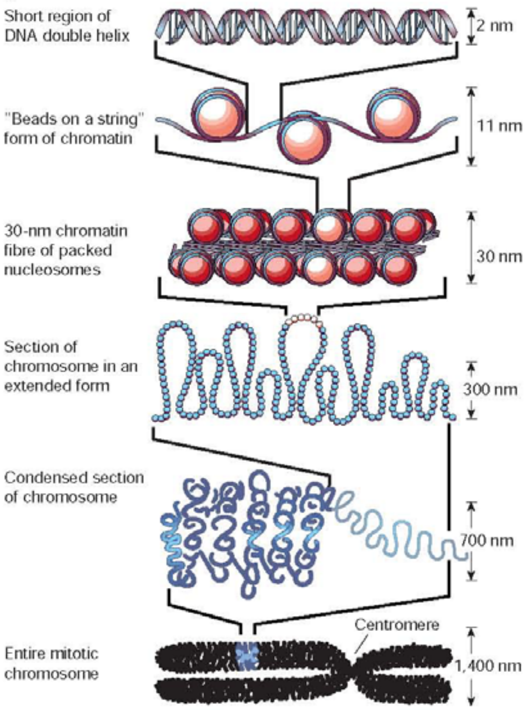

Fig. 2.5. Mesoscale biology. Mesoscale biology or "mesobiology" addresses structure and kinetic or dynamical processes at length scales of from a few to several hundred nanometers, which is the range in which much of the crucial biological activity takes place. [2.5] Cold neutron scattering experiments are particularly well matched to these biological length and time scales and can contribute to the fundamental understanding of the interplay between structure and process in such systems. (*Source*: G. Felsenfeld and M. Groudine, *Nature* **421**, 448–453, 2003).

2.1.6.2 Role of neutrons

Knowledge of the structure and dynamics of biological macromolecules is essential to the understanding of the functions of these macromolecules at the molecular level. However, the best single-crystal sample size is rarely above $100 \times 100 \times 100\ \mu m^3$ for these materials. Furthermore, the molecular weight of the protein determines the unit cell volume, which places limits on the molecular sizes that can currently be studied in such weakly scattering crystals. Forefront areas for neutron scattering studies include

- extending the utility of neutron protein crystallography by extending the instrumentation and the sample preparation capabilities to allow single-crystal structural studies of a much wider range of samples (e.g., high-data-rate, low-background neutron scattering instruments,

improved deuteration and crystallization capabilities), thus extending the knowledge of precise locations of functionally important protons to many more macromolecular systems
- lower-resolution structural measurements using high-intensity small-angle neutron scattering (SANS) with good signal-to-noise capabilities coupled with specific deuteration to provide information about the positions of individual residues on proteins and multi-component macromolecular structures in solution, and about the protein folding in solution
- using SANS to determine the kinetics, stoichiometry, and organization of large macromolecular complexes
- structural studies of membranes and the role of the polymer layer separating the biological membrane from the solid support
- structural studies of the association and self-assembly of functional clusters in the plane of the membrane
- extension of such measurements to study the membrane response to external stimuli such as drugs, pressure, etc.
- lipid dynamics in lipid bilayers and in lipid-water interfaces
- structures and kinetics of supramolecular complexes in oriented fibers, multilayers, and single monolayers
- structural studies of the hydration of macromolecules and the formation of solvation spheres around macromolecules in solution
- dynamical studies of the conformational flexibility of macromolecules
- dynamical measurements to verify and/or refine the inter-atomic potentials used in molecular dynamics simulations of biologically important macromolecules and macromolecular assemblies

2.1.7 Mineral Sciences, Earth Sciences, and Environment

2.1.7.1 Frontier research areas

Frontier research areas in mineral sciences and earth sciences include structural changes in minerals at very high pressures and temperatures; complex structures; polycrystalline aggregates under non-ambient conditions, including strain; and dynamical properties at non-ambient conditions. The physical and chemical properties of the minerals involved in the Earth’s crust and upper mantle are particularly important (Fig. 2.6), as is the role of water in these materials and related magmas (related to volcanic eruptions and earthquakes).

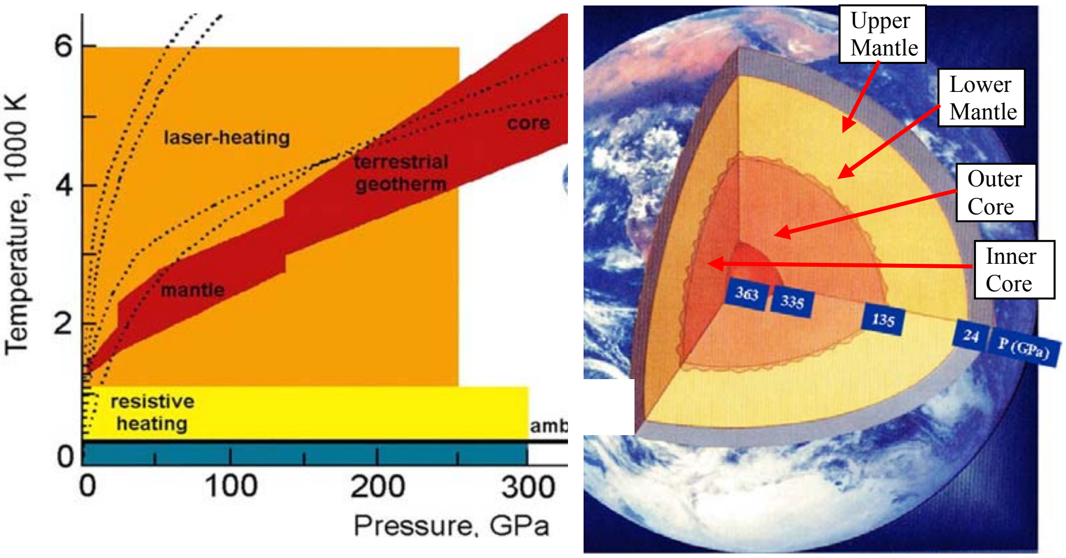

Fig. 2.6. Range of pressures and temperatures relevant to conditions within the Earth. Right: a cutaway of the Earth's interior. Left: the figure indicates the range of conditions that have been achieved in the laboratory. Neutron scattering can shed light on many geophysical processes, especially those in the crust and upper mantle. Much more intense neutron sources will enable scattering measurements to be made with much smaller samples, thus extending such measurements to processes and structures occurring deeper within the earth. (*Source*: H. Mao and R. Hemley, *PNAS* **104(**22), 9114–9115, 2007.)

2.1.7.2 Role of neutrons

Types of neutron scattering studies important to mineral science and earth science that could be done with improved neutron sources and instrumentation include

- structural and dynamic studies of pressure-induced spin dynamics and spin collapse in $Fe_xMg_{1-x}O$ and Fe_2SiO_4, as a mechanism for adaptation of simple crystal structures to high pressures (up to 100 GPa)
- in situ spectroscopic measurement of the molecular dynamics of water in nanoporous, hydrous, and nominally anhydrous mineral compounds at high pressure and temperature
- cation ordering at high pressure and temperature and the kinetics of associated phase transitions, accurate determination of the structures of pressure-stabilized gas hydrates and kinetics of their phase transitions, and in situ structural and dynamical studies of methane clathrates
- time-resolved neutron radiography and tomography to study the rheology and to address other physics and chemistry questions of fluids and melts at high pressures
- determination of the strain in each component phase of a rock aggregate under applied load, important to theories relevant to seismology
- texture measurements in large samples of polymineralic rocks
- in situ high-pressure and high-temperature studies of stress and strain partitioning and the development of textures in plastically deforming rocks

2.1.8 Fundamental Neutron Physics

2.1.8.1 Frontier neutron research areas

Forefront neutron experiments include

- two-body β-decay of unpolarized and polarized neutrons, to address the question of the origin of the "handedness" of nature
- gamma asymmetry in n-p and n-D capture
- neutron spin rotation in n-p and n-D reactions
- pushing the limits for measurements of the electric dipole moment of the neutron, relevant to the origin of the baryon asymmetry of the universe
- measurement of the neutron-neutron scattering cross-section
- neutron quantum optics
- neutron lifetime measurements

2.2 OTHER STUDIES

Two other recent studies have looked at the science cases for some types of facilities at pulsed sources or at steady-state sources. A recent workshop explored the scientific opportunities that would be made possible with a high-power very-cold-neutron source (VCNS) [2.5]. In addition, a workshop was held in the summer of 2006 to investigate the scientific opportunities and to help prioritize the instrumentation made possible by a second cold source and guide hall at the National Institute of Standards and Technology reactor [2.6]. The latter has some relevance to the SNS Second Target Station (STS) as well, even though it refers to opportunities at a steady-state rather than pulsed source. Neither of these studies is as extensive as those summarized in Sections 2.1.1 through 2.1.8. However, they offer examples of some additional specific scientific problems that could be addressed by the STS and are all in general agreement with the studies summarized in Section 2.1 as to what could be some of the forefront areas for scientific opportunities offered by an intense pulsed source of cold neutrons.

One further study that bears mentioning is the 2005 workshop "X-Rays and Neutrons: Essential Tools for Nanoscience Research" [2.7] held as part of the National Nanotechnology Workshop. This study focused specifically on the broad field of nanoscience and how neutron and X-ray measurements can contribute. That workshop emphasized that neutrons have a significant role to play in elucidating the fundamental interplay between structure and dynamics that determines the physical properties and functionality of nanoscale systems. It also set forth a road map indicating the need for new facilities and instrumentation and the time scale on which these must be brought on line in order to develop the full possibilities of "functionality by design" that could lead to a "nanotechnology revolution." Some of the specific types of experiments in which neutrons can make important contributions to nanoscience have already been outlined in Section 2.1.

2.3 IMPLICATIONS FOR THE SNS SECOND TARGET STATION

2.3.1 General Comments

Three major themes appear throughout the discussions of forefront science. The first is the desire to extend current capabilities to be able to answer more difficult questions. This extension of capabilities may involve taking measurements to higher resolution, performing the measurements in the presence of more difficult sample environments and concomitant restrictions to smaller samples, or measurements made to higher precision to look for subtle intensity variations or line shape effects. The second theme is the desire to extend most types of measurements to parametric studies exploring ranges of compositions, external fields such as temperature or pressure, or time scales, as in kinetic studies. The third theme is the general tendency toward the study of systems exhibiting greater complexity, such as the complex chemical systems that occur in many soft matter studies, the rapidly-expanding interest in using neutron scattering to probe aspects of macromolecular functionality important in biology, or the multi-component systems important to the geophysical properties and functions relevant to earth sciences.

Consequences of these themes are the desire to use smaller samples, the need to study weaker scattering processes, the need to extend structural and dynamical studies to investigate structures at longer length scales, the need to extend dynamical studies to probe slower motions (longer time scales), and the need to perform the measurements more rapidly in order to carry out real-time kinetics or relaxation experiments or to carry out extensive parametric studies. All of these lead to the requirement for higher neutron intensities—with a premium placed on the innovative use of neutron optics to enhance the flux on sample—and to the need for much higher intensities of longer-wavelength neutrons in order to probe materials and processes over longer length and time scales.

These trends are all evident currently as scientists stretch the capabilities of existing sources and instrumentation to try to extend their measurements into some of these areas. It seems almost certain that, regardless of which specific scientific problems move to the forefront in the future, these themes of greater difficulty, greater complexity, and parametric studies will continue in their prominence.

2.3.2 Specific Instrumentation Considerations

Table 2.1 summarizes the instrumentation identified in the workshops previously cited [2.1–2.3] as being necessary to carry out the full scientific agendas elucidated in Sections 2.1.1 through 2.1.8. Keep in mind, however, that this list of desired instruments is largely limited to minor extensions of instrumentation concepts that were well known at the time of the workshops. It does not take into account recent instrumentation advances that may provide new capabilities to address a few of the desired scientific studies that are not well addressed by the instrumentation suites listed (e.g., lateral structural measurements on surfaces). Bear in mind also that currently unanticipated innovative concepts that lead to new capabilities frequently can open up the field to totally new types of science. Thus, in conjunction with the construction of new facilities, it will be important to carry out a long-term robust program of neutron beam instrumentation development in order to fully realize the potential of these new high-intensity neutron sources.

As indicated in Table 2.1, a number of different scientific applications require some of the same instrumentation. This table also indicates that the current and planned instrumentation suite at the first (present) target station (FTS) will address a number of these instrumentation needs. However, many of the important instrumentation needs are either not addressed at all or else are only partially met with the FTS instrumentation suite. Therefore, there is a clear need for an STS that can address many of the remaining instrumentation requirements, and perhaps even extend the capabilities beyond what was envisioned at the time of the workshops cited [2.1–2.3].

2.3.3 SNS Second Target Station Requirements

Although the development of a second target station at SNS would roughly double the number of high-intensity beamlines available for neutron scattering, this in itself is not necessarily an adequate justification for building the STS. An overarching goal in the present exercise has been that a second SNS target station should enable new scientific opportunities—not just more of the same capabilities as found at the FTS. The analyses of the potential science opportunities and likely instrumentation needs presented led to the conclusion that the STS should focus on optimizing the flux of cold (long-wavelength) neutrons for a number of instruments. Since the FTS focused on short pulses, at the expense of maximum cold neutron flux, this would be an opportunity for the STS to offer capabilities in line with the scientific needs indicated earlier and complementary to the set of capabilities available at the FTS.

The basic requirements imposed on this exercise to define the STS were thus that it be designed to maximize the useful flux of cold neutrons to a number of instruments, and that the instruments at this station should be complementary to those at the FTS and should enable new scientific capabilities. The process to develop the concept for the STS followed this basic requirement. That process and the resulting facility concept are described in Chapter 3.

2.4 REFERENCES

2.1 The ESS Project, Vol. II, *New Science and Technology for the 21st Century,* The European Spallation Source Project, 2002. Available at http://neutron.neutron-eu.net/n_documentation/n_reports/n_ess_reports_and_more/102.

2.2 *Technical Concepts for a Long-Wavelength Target Station for the Spallation Neutron Source*, ANL-02/16, ORNL/SNS-TM-2001/163, November 2002.

2.3 *A Second Target Station at ISIS*, RAL-TR-2000-032, 2000. Available at http://ts-2.isis.rl.ac.uk/scienceCase/.

2.4 P. Ball, *Nature* **421**, 421–422, 2003.

2.5 *Proceedings of the Workshop on Applications of a Very Cold Neutron Source*, ANL-05/42, December 2005.

2.6 *NIST Second Cold Source and Guide Hall*. Report sections available at http://www.ncnr.nist.gov/expansion/NCNR_Expansion_Workshop_outcome.html

2.7 *X-Rays and Neutrons: Essential Tools for Nanoscience Research*, Proceedings of the National Nanotechnology Workshop, June 2005, to be published.

Table 2.1. Neutron beam instrumentation required for next-generation science

Type	Instrument	Section requesting instrument							
		2.1.1	2.1.2	2.1.3	2.1.4	2.1.5	2.1.6	2.1.7	2.1.8
SANS									
	High-resolution focusing small-angle-scattering instrument		X	X	X				
	High-intensity SANS			X	X	X			
	High-resolution SANS optimized for biology						X		
	High-intensity SANS optimized for biology						X		
Reflectometry									
	Polarized neutron reflectometer with high Q resolution and high intensity		X	X					
	High-intensity reflectometer			X	X				
Diffraction									
	Powder diffractometer with 0.1% d resolution	X	X	X					
	High-intensity powder diffractometer	X	X	X					
	Engineering diffractometer for stress-strain analysis		X						
	Diffuse scattering diffractometer with full polarization analysis		X		X				
	Good-resolution powder diffractometer covering length scales of up to a nm	X	X	X	X				
	Small-unit-cell single-crystal diffractometer	X		X					
	Magnetic powder diffractometer	X	X	X					
	Single-pulse diffractometer		X	X					
	Liquids diffractometer				X	X			
	Intense, focused-beam protein crystallography diffractometer for small crystals						X		
	Intense, larger-beam long-wavelength crystallography diffractometer for higher-molecular weight crystals at high resolution						X		

Table 2.1 (continued)

Type	Instrument	Section Requesting Instrument							
		2.1.1	2.1.2	2.1.3	2.1.4	2.1.5	2.1.6	2.1.7	2.1.8
Diffraction (cont.)									
	Extreme environment diffractometer(s) for high pressure and temperature							X	
	Instrument to perform simultaneous phase, structure, texture, and stress analyses under high-pressure and -temperature conditions							X	
Inelastic Scattering									
	High-resolution backscattering spectrometer	X	X	X	X	X	X		
	Lower-resolution backscattering spectrometer with Q of up to 5 Å^{-1}	X					X		
	Variable-resolution cold neutron chopper spectrometer	X	X	X	X	X	X		
	Thermal chopper spectrometer	X		X		X	X		
	High-energy chopper spectrometer	X		X		X			
	High-resolution neutron spin-echo spectrometer			X	X	X	X		
	Wide-angle spin-echo spectrometer				X	X	X		
	One or more inelastic spectrometers dedicated to (or at least useable for) ultra-high pressure and temperature measurements							X	
Imaging									
	Tomography and radiography instrument using time-of-flight to identify different components and phases		X					X	
Fundamental Neutron Physics									
	Beamline dedicated to ultra-cold neutron production								X
	Beamline for neutron decay studies								X

Table 2.1 (continued)

Type	**Instrument**	**Section Requesting Instrument**							
		2.1.1	**2.1.2**	**2.1.3**	**2.1.4**	**2.1.5**	**2.1.6**	**2.1.7**	**2.1.8**
Fundamental Neutron Physics (cont.)									
	Cold beamline for neutron optics studies including interferometry								**X**

🟦 An instrument at the FTS is available or is being built to satisfy most of these requirements.

X Instrument requested in Sections 2.1.1 through 2.1.8

3.0 FACILITY CONCEPT

3.1 PROCESS FOR DEVELOPING A REFERENCE CONCEPT FOR AND EVALUATING THE PERFORMANCE OF THE STS

3.1.1 Outline of Process

The process for developing the results presented in this report followed these steps:

1. Basic assumptions: The STS facility should be science-driven and complementary to the FTS.
2. Scoping workshop: A scoping workshop to kick off the planning effort to develop the STS was held on August 3–4, 2006, at the SNS, with the goal of defining some of the basic performance parameters for this target station.
3. Initial accelerator study: The workshop was followed by a study to define the capabilities and options offered for the STS by the SNS accelerator systems.
4. Neutronics workshop: A workshop was held December 14–15, 2006, to develop a neutronic design for the STS target station, consistent with the outcomes of the scoping workshop and the accelerator study.
5. Initial neutronics study: The design concept developed in this neutronics workshop was incorporated into an initial neutronics model for the STS target station, and an initial set of neutron production performance calculations was carried out.
6. Instrumentation workshop: This calculated neutronic performance served as input for an STS instrumentation workshop that was held February 20–22, 2007, at the SNS. This workshop focused on instrumentation suitable for the calculated STS source performance and provided feedback for optimizing the neutronic performance.
7. STS working group: An STS working group was formed to meet regularly to assess the information generated in steps 1–6 and to generate from it a reference facility concept and an assessment of the scientific impact of such an STS. The output of this working group is presented in this report.

Each of these steps is elaborated in the following subsections.

3.1.2 Basic Assumptions

The current effort to develop the concept for a second target station at the SNS began in the summer of 2006. The overall constraints imposed on this effort followed from the scientific considerations presented in Chapter 2. These constraints were that this target station should be optimized to maximize the useful flux of cold neutrons to a number of instruments, and that the instruments at this station should be complementary to those at FTS and should enable new scientific capabilities.

3.1.3 Scoping Workshop

A scoping workshop (~35 local and international experts) was held on August 3–4, 2006, at SNS to kick off the effort to develop a concept for the STS , with the goal of defining some of the basic performance parameters for the target station and clarifying the next steps to be taken in this process. Some very high-level questions were addressed, including whether the second target station should be a long-proton-pulse source (proton pulse duration delivered to target station of ≥ 1 ms) or short-proton-pulse source (proton pulse duration delivered to target station of ~ 1 μs, as for the first target station) and whether the effort should be made to produce much colder spectra than typically available at cold neutron sources to date. This was a true "workshop" with no formal presentations and with the discussions taking place in working groups organized around scientific areas to identify gaps in current capabilities, potential types of instrumentation to fill these gaps, and the source performance parameters required to implement such instrumentation. Results from this workshop are summarized in a report [3.1].

Consensus conclusions of the working groups were that

- The STS should focus on achieving the highest practical usable flux of cold neutrons by making all the moderators cold coupled moderators.
- The STS should operate at no more than 20 Hz.
- Either short proton pulses or long proton pulses can be used for the STS and both should be considered.
- A VCNS moderator could be considered for one, but not all, of the moderators on the STS.
- The STS must be able to achieve highly reliable (90%) operation in order to be useful as a user-based facility.

3.1.4 Initial Accelerator Systems Study

Following the scoping workshop, a team of SNS accelerator physicists and system experts was asked to explore the options for feeding intense pulsed proton beams to a second target station (in addition to the one already operational). This team investigated a number of issues, including the long-proton-pulse versus short-proton-pulse question and the operating frequency issues raised in the scoping workshop. They also looked briefly into options for further increases in the total power output by the SNS accelerator systems (beyond the increases already planned as part of the SNS PUP), since such increases would permit the delivery of more power to the second target station. This team defined a number of options and provided very rough cost estimates for each of these options. This preliminary work is summarized in a report [3.2].

3.1.5 Neutronics Workshop

A neutronics workshop (~20 local and international experts) was held December 14–15, 2006, at SNS to follow up on some of the source-configuration questions raised at the scoping workshop and to define the most promising target-moderator-reflector configurations for additional studies by the SNS neutronics group. The conclusions from this workshop were as follows (G. Bauer, FZ-Juelich. Personal communication to R. K. Crawford, ORNL, 2007):

- We should focus on a coupled target-moderator-reflector system.
- We should plan on a 1 MW system with a capability to upgrade to ~3 MW (so bulk shield, non-upgradeable utilities, etc. must be planned for 3 MW).
- The short-proton-pulse versus long-proton-pulse issue is still open. There may be advantages to running a coupled moderator system in short-pulse mode at 1 MW of beam power.
- Short-proton-pulse injection into a coupled system gives better performance for some types of instruments (at a constant number of protons per pulse and the same target-moderator configuration), whereas for other types of instruments, there is no difference in performance between short-proton-pulse and long-proton-pulse injection.

3.1.6 Initial Neutronics Study

Following the neutronics workshop, the SNS neutronics group carried out performance calculations and optimizations for the target-moderator-reflector geometry recommended in the neutronics workshop. This model was a large fully coupled parahydrogen moderator in wing geometry above the target and viewed by multiple beamlines. This model allows a similar moderator to be located below the target, so the number of beamlines could be doubled. The calculated performance from this system was quite good, with time-averaged neutron intensities per proton of about three times the corresponding quantities for the FTS coupled parahydrogen moderators and with even greater gains for peak intensities. Greater detail concerning these preliminary calculations was made available in a draft report [3.3].

3.1.7 Instrumentation Workshop

An instrumentation workshop was held at the SNS on February 20–22, 2007, to explore and evaluate neutron beam instrumentation that would perform well with the preliminary source performance parameters developed in the accelerator and neutron source studies discussed in Sections 3.1.3 through 3.1.6. Approximately 70 national and international experts participated in this workshop. One goal specified for this instrumentation workshop was to provide input for a reference list of instruments (or other beamline uses) that have significant scientific potential and would utilize the unique source characteristics of the STS. An important aspect of this process was to identify the source characteristics important to the performance of each instrument (e.g., short vs long proton pulse, neutron energy spectrum) so that this information could be used in subsequent further refinement of target, moderator, and accelerator parameters. There were few formal presentations at this workshop; most of the workshop was devoted to parallel sessions of working groups made up of subject matter experts focused on particular types of neutron beam instrumentation. The number of working groups and the membership of each were designed to cover the entire range of instrumentation types anticipated.

The working groups assessed more than 40 specific neutron scattering instruments or other neutron beam applications. A few of these were found to perform better on the FTS or at the High Flux Isotope Reactor (HFIR) neutron scattering facility, but nearly 30 of the instruments appeared to be reasonable candidates for the STS. Each working group produced a report containing its “straw man” instrument list, including instrument-specific information and any other supporting information. These individual working group reports were combined into a workshop report [3.4].

3.1.8 STS Working Group and Follow-up Analyses

Following these workshops, an STS Working Group was established to synthesize the information generated in the workshops and preliminary reports and to develop and evaluate a concept for a second target station at SNS. This working group provided direction for subsequent analyses to be performed, leading to the selection of a "reference concept" for the STS and the evaluation of the performance to be expected from this reference concept. This working group, made up of representatives of the SNS scientists, engineers, neutronics team, accelerator systems, and site facilities, also was responsible for assembling the resulting material into this white paper. This reference concept for the STS facility is presented in the remainder of Chapter 3; Chapter 4 summarizes the performance evaluated for this reference concept for the STS.

Section 3.2 sets out the baseline choices that came out of the deliberations of the STS Working Group, along with the reasons for those choices. Sections 3.3 and 3.4 describe the concepts for the accelerator modifications and for the second target station design that flow from these baseline choices. Section 3.4 also summarizes the neutronic calculations used for the preliminary optimization of the design for this target station and for evaluating the neutronic performance of the STS facility. Section 3.5 presents a "reference instrument suite" of 20 concepts for neutron beam instruments and a high-level performance assessment for each of these instruments, based on the source performance defined in Sects. 3.3 and 3.4. Finally, Sect. 3.6 provides a layout of the entire STS facility, including the proton beam transport line, the target station and target building, the additional required infrastructure, and the reference instrument suite.

3.2 BASELINE CONFIGURATION FOR THE STS REFERENCE CONCEPT

The results of the process described in Sect. 3.1 led to the following choices for the baseline configuration assumed for the STS reference concept presented in this report. A further requirement driving the choices made for the baseline configuration was that the technical risk in implementing the resulting configuration be relatively low. A concept optimization program (including some research and development [R&D]) proposed in Chapter 6 is aimed at further conceptual design optimization (beyond this baseline configuration) of the performance, reliability, cost, and/or schedule for the facility. The major parts of this baseline configuration and the reasons for the choices made are discussed in this section.

3.2.1 Accelerator Systems Capabilities Assumed for the STS

3.2.1.1 Beam power

- The baseline accelerator systems will provide at least 1 MW at 40 Hz to the FTS and ~1 MW at 20 Hz to the STS.

An accelerator system capable of delivering 2 MW total at 60 Hz is promised as part of the PUP baseline. The PUP internal goal is to provide 3 MW, which would leave up to an additional 1 MW to be distributed as appropriate between the FTS and the STS. The 20 Hz operating frequency for the STS is chosen to provide reasonable usable bandwidth for the relatively long instrument beamlines required because of the long neutron pulse widths at the STS.

3.2.1.2 Operating mode

- Protons will be delivered to the STS in long-proton-pulse mode (no accumulation in the ring), resulting in proton beam pulses ~1 ms long. The proton beam will not be chopped for the long-pulse-mode pulses, leading to ~50% more power to the STS.

Up to 50% more total proton beam power can be provided in the long-proton-pulse mode than in the short-proton-pulse mode. The reason is that the long-proton-pulse mode does not require chopping out parts (~1/3) of the proton beam, a step necessary to store the protons for many turns in the ring and then extract them cleanly in a single turn. Therefore, the parts of the proton beam that would be chopped out in short-proton-pulse mode can be delivered with the rest of the beam to the target in long-proton-pulse mode, resulting in a significant gain in neutron production. This can be done with the same accelerator system ion source and duty cycle capabilities, requiring only some upgrades in the RF, SCL cavity cooling, SCL cavity coupler, and High Voltage Converter Modulator (HVCM) systems.

Most of the instruments that would be used at the STS can operate equally well or nearly as well in long-proton-pulse mode as in short proton-pulse mode, even at the same total beam power (see Sect. 3.5). This increase of power by up to 50% in long-proton-proton-pulse mode operation tips the scale strongly in favor of long-proton-pulse mode for maximizing the combined capabilities of the suite of STS instruments.

In addition, long-proton-pulse mode does not require storing the beam in the accumulator ring, where higher numbers of protons per pulse can lead to unacceptably high losses and consequent restrictions on the total power per pulse.

Finally, in long-proton-pulse mode, the proton beam energy is not as concentrated in time as it is in short-proton-pulse mode, resulting in opportunities for further optimization of the target-moderator-reflector configuration that lead to additional increases in the neutron beam intensities.

As a further consideration, upgrade paths are foreseen that could lead to even higher proton beam powers being delivered by the linac. However, the accumulator ring could not handle these higher powers, so such an additional power upgrade could apply only to beam produced in the long-proton-pulse mode.

3.2.1.3 Operating frequency

- The accelerator systems will run at 60 Hz with every third pulse going to the STS and the other two-thirds of the pulses going to the FTS.

This “pulse-stealing” mode (40 pulses per second at the FTS and 20 pulses per second at the STS) at 2 MW and equal power per pulse will result in 1.33 MW to the FTS and 0.67 MW to the STS (increasing to ~1 MW on the STS in long-proton-pulse mode with no proton beam chopping). In this mode, the intervals between successive pulses at the FTS will be in the sequence 16.7–33.3–16.7–33 ms …, whereas the STS pulses will be at a true 20 Hz with 50 ms spacing between pulses.

An alternative higher-frequency operating mode delivering 60 evenly spaced pulses per second to the FTS, with an additional 20 evenly spaced pulses per second to the STS interleaved between these, will be analyzed as part of the concept optimization program. In this mode the same total power on the FTS can be achieved with less power per pulse, resulting in lower stress on the mercury target and lower beam losses in the ring. This could become particularly important when the linac ramps closer to full power goals, providing more beam power than the 2 MW that is the official PUP baseline (internal PUP goals are up to 3 MW). It would also avoid the potential variability of pulse-to-pulse backgrounds at the instruments that result from non-uniform spacings between the FTS pulses in the pulse-stealing mode.

The higher-frequency operation has relatively low technical risk, but it is expensive in terms of both initial capital costs and operating costs because of higher power consumption. Therefore the pulse-stealing mode has been chosen as the baseline for the reference concept.

3.2.1.4 Beam transport

- A portion of the ring and the present area for extracting beam from the ring will be used as part of the proton transport line to the STS in long-proton-pulse mode.

The present SNS site configuration precludes the straightforward use of a long-proton-pulse beamline that bypasses the ring entirely and goes directly from the linac to the STS target. Although the transport of the long pulse through the ring is straightforward, such a direct transport line would be highly desirable from a facility maintenance and operational availability perspective (e.g., to keep the STS operating while maintenance is being performed in the ring). Therefore, continued exploration of the possibilities for providing such a direct beam transport line will be part of the concept optimization program planned as further optimization of the conceptual design for this project.

3.2.2 Target Station for the STS

3.2.2.1 Design power

- The target station will be designed to operate at up to 3 MW to accommodate potential future linac upgrades. The monolith shielding and other non-replaceable systems will be installed to handle 3 MW, whereas replaceable systems and shielding will be installed to handle 1 MW.

Although the baseline plan is for 1 MW on the STS target, there appears to be no fundamental technical issue preventing a later upgrade of the linac to provide higher power in long-proton-pulse mode. Therefore, it is best to plan for this eventuality when the STS is built (i.e., in the same spirit that the FTS target station and non-replaceable infrastructure were designed from the outset to accommodate 2 MW even though the initial SNS internal baseline was only 1.4 MW).

3.2.2.2 Target material

- The target will be flowing mercury, and the vessel will be similar to that on the FTS.

In long-proton-pulse mode, there should not be any serious mercury cavitation problems, so the mercury target should be a relatively conservative choice for 1 MW. There is a reasonable chance that mercury would continue to be a viable choice at the 3 MW level in long-proton-pulse mode. Furthermore, safety and other issues associated with operation of a mercury target have already been addressed for the FTS, and there will be a wealth of operating experience by the time the STS is built. Nevertheless, the proposed concept optimization program (see Chapter 6) would investigate other target options as further optimizations of the conceptual design.

3.2.2.3 Moderators

- There will be two large cylindrical wing moderators, one above and one below the target, filled with a controlled mixture of ortho and para hydrogen. Neutron beams will be extracted through several openings in the reflector surrounding these moderators. One or more of these openings may view a beryllium filter-reflector on the outer face of the moderator to provide a colder spectrum.

This combination provides the highest time-averaged intensity of cold neutrons simultaneously for a number of neutron beams of all the configurations so far investigated. Other options will be considered in further optimizations of the conceptual design, to be carried out as part of the concept optimization program (see Chapter 6).

- Each of these moderators will feed ten or more neutron beamlines.

Ten appears to be the maximum number that can reasonably be brought out without opening up the aperture through the reflector too wide and while still providing enough separation between beams to permit operation of pulse-shaping or bandwidth choppers reasonably close to the moderator (6–9 m). Other configurations will continue to be investigated in further optimizations of the conceptual design, to be carried out as part of the concept optimization program (see Chapter 6).

3.2.2.4 Neutron beams

- All neutron beams will have neutron guides that penetrate as closely as practical to the moderators.

Having the guides start close to the moderator provides significant gain, especially for cold neutrons.

- There will be no individual-beam “primary shutters” (similar to those on the FTS) within the target station shielding monolith. Every neutron beam will have its individual “secondary shutter” at some point outside the target station shielding monolith.

The elimination of primary shutters will greatly simplify the design and construction of the target station shielding monolith. This arrangement requires that remote handling be used for all maintenance and repair operations on the beamline components upstream from this secondary shutter. Optimal methods for such remote handling will be explored as part of the program for further optimization of the conceptual design (see Chapter 6).

Most of the neutron beams will be curved or will have benders so that most of the instrument can be placed beyond the line-of-sight for fast neutrons. In most cases, the secondary shutter will be placed beyond this line-of-sight point so that only a minimal shutter is required to stop the remaining thermal and cold neutrons in the beam.

- The facility will be designed with an arrangement to block the residual gamma radiation and/or to provide remote handling capabilities to allow installation/maintenance access to the inner guide sections and the choppers during facility shutdown periods.

  See discussion for previous bullet.

- Not all of the beamlines will be instrumented initially, so it will be necessary to provide shielding plugs and/or additional temporary shielding to block radiation from the uninstrumented beamlines.

As at the FTS, not all the beamlines will be instrumented when the STS starts operation. This is a desirable situation, since it leaves open the possibility for a phased development of new methods and technologies designed to meet changing scientific needs as the full instrument suite is being completed over time. Furthermore, limited resources such as floor space and crane availability make it impractical to install all 20 or more instruments concurrently.

3.2.3 Instruments for the STS

- All STS instrument beamlines must fit within the area defined by the existing elliptical perimeter road and the FTS target building and instrument beamlines.

The elevation of the terrain at the Chestnut Ridge SNS site falls off very rapidly outside the perimeter road, making the extension of neutron beamlines beyond these limits technically problematic and/or prohibitively costly.

3.2.4 Conventional Construction Required for the STS

3.2.4.1 Target building

- The STS target building will be sited close to the elliptical perimeter road in an orientation that permits several beamlines to have maximum lengths of ~130 m.

Locations in this general area provide options for some long beamlines with minimum interference with the FTS and its instruments. Several of the STS reference instruments require such long beamlines to achieve the required time-of-flight (TOF) resolution with the broad STS pulses.

- The STS target building will be slightly larger than but otherwise similar to the FTS target building, with a few exceptions.

The design for 3 MW will require a somewhat larger diameter of the target monolith shield, which in turn requires a greater width for the high bay over it. There will be more headroom and a 100-ton crane in the high bay to allow other simplifications in the target station design and to facilitate remote handling for maintenance operations. The target service bay will be located downstream from the target position, as at the FTS, but this service bay will be wider than the one on the FTS. The target building itself will be a little wider than the present target building to accommodate more of the instruments inside the building. Non-replaceable utilities installed in the target station, service bay, and target building will be sized for 3 MW.

- The STS target station will be asymmetrically located inside the target building.

This location will provide room for short (30–50 m) instruments to fit inside the building on the side facing the elliptical road.

3.2.4.2 Offices and laboratories

- Another office-laboratory building or buildings will be required to provide ~200 additional offices plus some laboratories to house the additional staff required to operate the STS and the users who will be present during operation.

This assumes 20 beamlines with 6 staff per beamline (= 120). It also assumes offices plus some technician space for the target station and building operations staff and system experts and assumes a number of users comparable to the FTS at fully instrumented operation.

3.2.4.3 Proton transport tunnel

- A tunnel will be required for the proton transport line. This tunnel will connect between the present Ring to Target Beam Transport (RTBT) tunnel and the STS target station and will have similar requirements, including utilities, to those for the present High Energy Beam Transport (HEBT) and RTBT tunnels.

3.2.4.4 Infrastructure

- Infrastructure upgrades/additions are required to support the new STS facilities (e.g., added RF power, second target building and instruments, beam transport tunnel, new office building). This new infrastructure includes the following:
  - Additional water tower
  - Additional cooling tower
  - Additional electrical power capacity
  - Additional Central Utilities Building
  - Road access to target building
  - Distribution of all utilities to the STS proton transport line and to the target building

3.3 ACCELERATOR SYSTEMS

3.3.1 Present SNS Accelerator Systems

The SNS Construction Project requirements call for the SNS accelerator to provide ≥ 1 MW of proton power on the FTS target in short-proton-pulse mode at 60 Hz [3.5]. However, the internal project goal is to provide 1.4 MW of proton power to the FTS target station, and the present design and installed capabilities are intended to support this goal [3.6]. In particular, the goal is for the SNS accelerator to provide 1.4 MW by accelerating a 38 mA beam to 1 GeV with a 1 ms pulse length in the linac. The linac output beam is accumulated in the storage ring for 1060 turns, compressing the beam in preparation for fast extraction. A single turn extraction provides a short pulse (< 1 μs) beam on the target, with the entire process occurring at 60 Hz. The main accelerator parameters for the SNS baseline and the other cases discussed here are shown in Table 3.1.

Table 3.1. Parameter comparison of SNS baseline, power upgrade project, and STS options

	Baseline SNS	**Baseline PUP (internal goal)**	**Baseline two target stations**	
			FTS	STS
Beam power on target (MW)	1.4	2 (3)	1.33	1
Beam energy (GeV)	1	1.3	1.3	1.3
Beam rep. rate (Hz)	60	60	40	20
Charge/pulse accelerated (μC)[*]	26	28 (42)	28	42
Energy/pulse on target (J)	24	33 (50)	33	50
Macro pulse length (msec)	1.0	1.0	1.0	1.0
Peak macropulse H-current (mA)	38	43 (59)	43	43
Linac chopping fraction	0.68	0.72	0.67	1.0
Injected turns	1060	1000 (1080)	1076	

[*] Assumes 5% injection stripping loss and 5% of the beam misses the target.

3.3.2 Power Upgrade Project

The PUP [3.7] proposed for the SNS has an approved CD-0 mission statement to provide >2 MW proton power on the first target. The baseline accelerator parameters for this project could provide a beam power of up to 3 MW. The power increase is accomplished by increasing the beam energy from 1 to 1.3 GeV and increasing the beam current by 60%. The PUP strategy does not include provisions for increasing the linac duty factor. The beam energy increase is accomplished by adding additional superconducting cryomodules in existing vacant linac space reserved for this purpose. The increase in beam current is accomplished by the development of higher-performance ion sources. Some additional PUP accelerator impacts include enhancements of the RF system needed to handle the increased beam loading corresponding to the higher current, modification of some ring injection magnets to handle the higher energy, and R&D on the stripper foil in the ring injection to handle the higher power.

3.3.3 Additional Modifications Required for the STS

3.3.3.1 General requirements

The baseline operational mode for the STS is the “pulse stealing” mode, which is possible using the PUP beam parameters. In this mode, the FTS target station would operate at up to 2 MW and 40 unevenly spaced pulses per second, and the STS would operate at 20 Hz and at least 1 MW. The pulse stealing option requires 50% higher power per pulse to the FTS to achieve the same total power as for 2 MW 60 Hz FTS operation, but this would be possible with the 3 MW PUP beam parameters with no additional accelerator development costs other than the new beam transport line.

An alternative mode of operation is to maintain a short-proton-pulse beam at 60 Hz and up to 2 MW on the FTS target and to provide an additional 1 MW beam with interleaved pulses at 20 Hz to the STS target (see Sect. 3.2.1.3). This requires an increased duty factor for the accelerator, and the accelerator implications for this scenario are non-trivial. The RF system might have to operate at 120 Hz to accommodate the 60 Hz equally spaced pulses to the FTS and an additional 20 Hz equally spaced pulses to the STS. Increasing the RF system to operate at higher frequencies may require significant rework of the linac, as discussed in Sect. 6.1. There are some potential performance advantages to this mode, but the amount of rework required and the cost that would entail keep this from being the baseline choice. However, further study of this mode is warranted and is proposed as part of the concept optimization program in Chapter 6.

For either of the STS beam delivery modes, the intent is ultimately to be able to deliver 3 MW of proton beam at some appropriate distribution between the FTS and the STS, since this is the upper range of the expected accelerator capabilities after the PUP upgrade.

3.3.3.2 Additional requirements for long-proton-pulse beam operation

The baseline for the STS reference concept is delivery of the beam in long-proton-pulse mode (~1 ms). This would be accomplished by not storing the beam in the accumulator ring but rather transporting the beam directly from the linac to the STS, using a portion of the ring as a transport line. This arrangement requires adding at least two pulsed ring magnets that would divert the beam to the ring extraction septum during the STS pulses only. These magnets would be similar to the eight existing injection kicker magnets used to paint the injected beam in the ring.

The STS reference concept baseline also calls for the chopping of the proton beam to be turned off during the preparation of these long pulses. Discontinuing chopping provides ~50% more time-averaged current at the same duty factor for the RF and the ion source. It does require more power to the RF because of the increased beam loading, but is cost-effective because of the resulting ~50% increase in total power made available to the STS.

Long-proton-pulse operation for the STS could have another large impact on the beam power delivered to the STS. A key consideration in the ultimate beam power possible for the FTS and the STS is the tolerable beam loss in the ring. For short-pulse beam delivery, the ring is required to store an extremely high-intensity beam, which occupies much of the available aperture. Injection, storage, and extraction of such a high-intensity beam are more problematic than simply transporting the beam directly from the linac to a target; and beam loss issues associated with the high-intensity beam storage will ultimately limit the SNS power in short-proton-pulse mode. With long-pulse beam delivery, these problems should be alleviated. Although it is difficult to predict exactly how much more beam could be delivered in long-pulse mode for the same beam loss as in short-pulse mode, it is likely to be at least 10s of percent more.

3.4 TARGET STATION CONCEPT

3.4.1 Introduction and General Configuration

The design concept for the second target station is based on the requirements for the neutron scattering instruments along with the experience and lessons learned from the first target station at SNS. Figure 3.1 shows the overall arrangement of the proposed building.

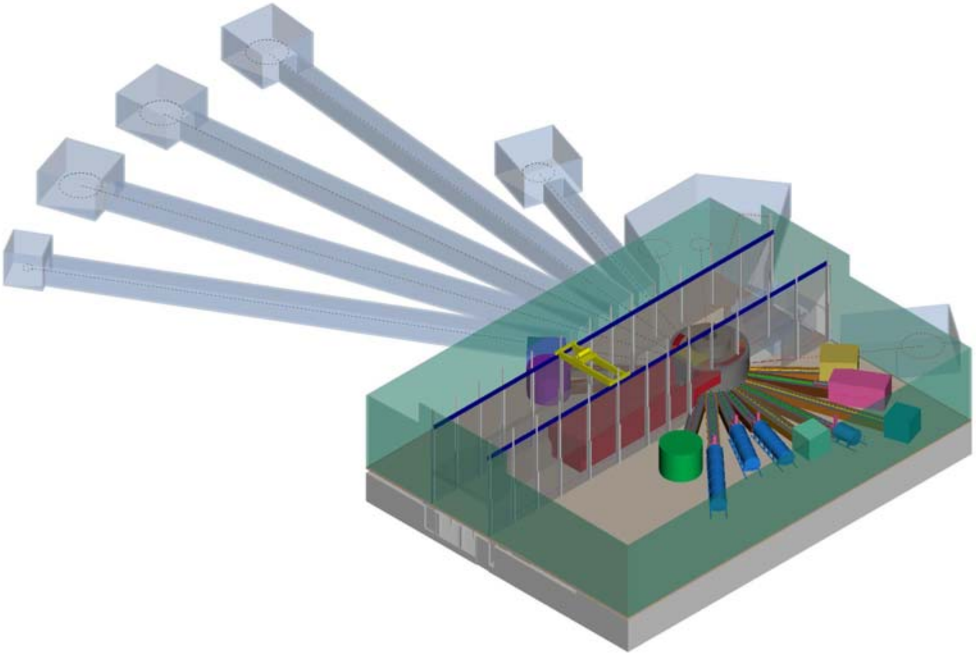

Fig 3.1 Proposed STS target building.

The arrangement of the proposed facility is similar to that of all recent spallation facilities—a horizontal proton beam colliding with a target located in the center of an iron and high-density-concrete shielding monolith. Ten neutron beamlines will array on each side of the monolith, illuminated by two large supercritical, coupled-hydrogen moderators above and below the target. A shielded target service bay (TSB) used to replace the targets and contain the mercury cooling loop will be located downstream of the proton beam. The overall building length will be 90 m. The center of the monolith is closer to the side where instruments will be located outside the target building on long beam lines. The overall building width was increased from 61 to 68 m to provide more space on the opposite side where instruments need to fit within the building. Basement areas will house the water cooling loops, ventilation systems, personnel facilities, and other similar utilities and services. Figure 3.2 shows a plan view of the proposed building at the instrument floor level.

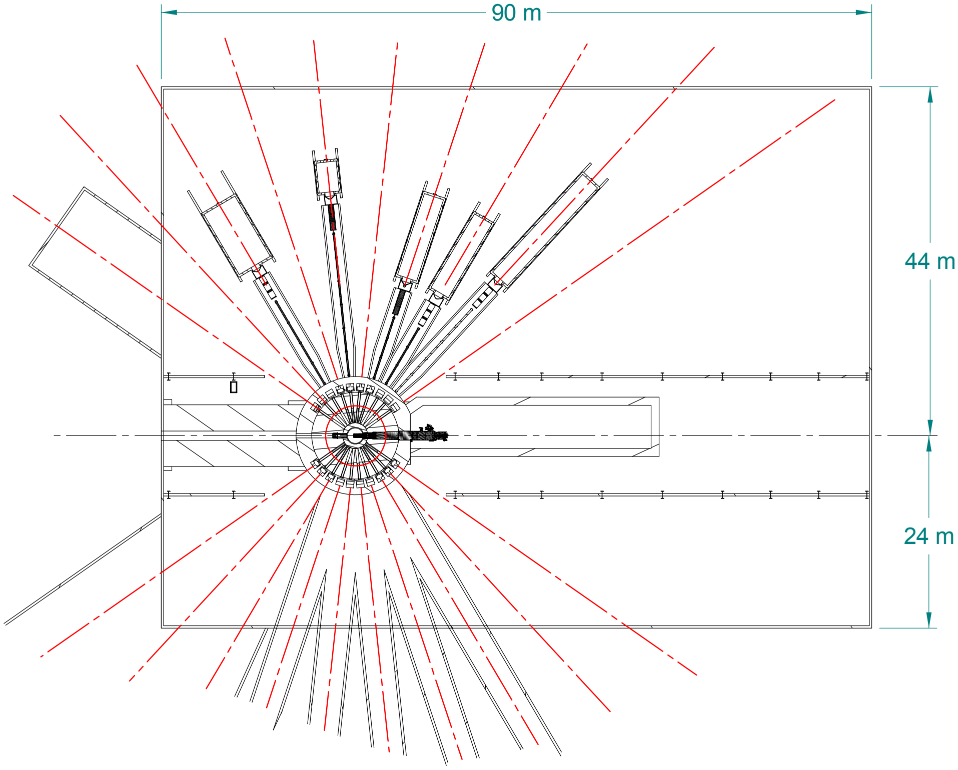

Fig. 3.2. Target building plan view.

The proposed monolith shielding will be thicker than for the FTS (7.5 m radius vs 6 m) (see following section). This increase leads to a wider and more useful central corridor. Based on installation and operating experience with the mercury system in the first TSB, the width of the service bay was increased from 4.3 to 5.5 m to provide more room for equipment, access for maintenance, and laydown space. The general arrangement for process equipment and target carriage is expected to be similar to that for the FTS.

A significant difference between the proposed STS and the FTS will be the use of curved neutron beam guides instead of primary shutters within the monolith. These allow for a less complex design for the monolith shielding and a more efficient use of iron shielding.

3.4.2 Neutronic Performance and Shielding

Scoping studies were performed to evaluate the performance of various moderator geometries, including slab, wing, flux trap, and large-volume wing moderators, as well as the impact of beryllium reflector/filters for each geometry. These studies were carried out using the Monte Carlo program MCNPX. The importance of comparing each of these geometries in an optimum configuration necessitated automating an optimization routine based on a quantifiable metric. This initial study used the crude metric of neutron brightness integrated over wavelengths greater than 4 Å for a 10 cm wide by 12 cm tall field of view extracted from a minimum of 20 beamlines.

Because the moderators are optimized for high-intensity long-wavelength neutron beams, the moderators are fully coupled and premoderated. With this configuration, the pulse lengths of the neutron beams are long compared with those in decoupled systems. Because the pulse lengths are fundamentally long, the optimized moderator configurations can be significantly larger in size and subsequently in volume than are typical moderators at existing facilities, without a significant negative impact on instrument resolution.

The optimization studies focused on liquid hydrogen and liquid deuterium as moderating materials because these are known not to degrade in severe radiation fields of megawatt-level facilities. The liquid hydrogen ortho-hydrogen fraction was allowed to vary in the search for an optimized moderator system. The results, consistent with previous studies in the literature, indicated that large parahydrogen moderators resulted in the highest long-wavelength brightness from a pulsed spallation source target system.

Both lead and beryllium reflector systems were considered in the studies. Large-volume moderators are primarily target fed, and the reflector plays a secondary role. Little difference was seen between a beryllium and a lead reflector in the configurations studied; there was a slight time-averaged gain for the beryllium reflector. In addition, the engineering complications introduced by a lead system favor the choice of beryllium for the reflector system, which we adopted for the final configurations.

The results of the optimization study (shown in Fig. 3.3) indicated that a slight advantage, less than 10%, could be achieved for cold neutrons feeding into the near-normal beamlines when a slab moderator configuration is used. For comparison purposes, the neutron brightness for each configuration is shown relative to the existing SNS target station in Fig. 3.4, which shows that the neutron brightness for both the slab and the volume wing configurations are approximately 5.5 times greater than for the existing SNS target station (even more at longer wavelengths). However, this slab gain is lost as the viewing angle becomes large, as shown in Fig. 3.5, with performance eventually favoring the volume wing moderators. For this reason, the useful viewing angle for slab moderators is limited, and a second, lower-intensity moderator is needed for additional beamlines. When a volume wing moderator is used, all beamlines view the highest-intensity moderator. Additionally, the high-energy flux component emitted into beamlines fed by wing moderators is significantly suppressed compared with that emitted into beamlines with slab moderator configurations. This suppression may not be of much importance to neutron background in curved guide systems, but it may impact the lifetime of beamline components near the target, such as neutron choppers, guides, and benders. For these reasons, the initial design concept settled on large volume wing moderators.

Shielding of the target system will be sized for 3 MW beam operation. The size of the shielding monolith, both height and radius, was based on calculations completed for the existing SNS target station. The height of the iron region has been increased slightly to account for the increased power, and the radius has been increased significantly to account for the fact that plans do not call for repeating the existing chopper column design on the second target station. Whereas the target monolith will be sized at a radius of 7.5 m, the first chopper void for each beamline will be located inside the monolith at a distance of approximately 6.5 m. With the chopper voids inside the monolith, the effective increase in shielding is smaller than the difference between 7.5 m for the STS and 6 m for the FTS may indicate.

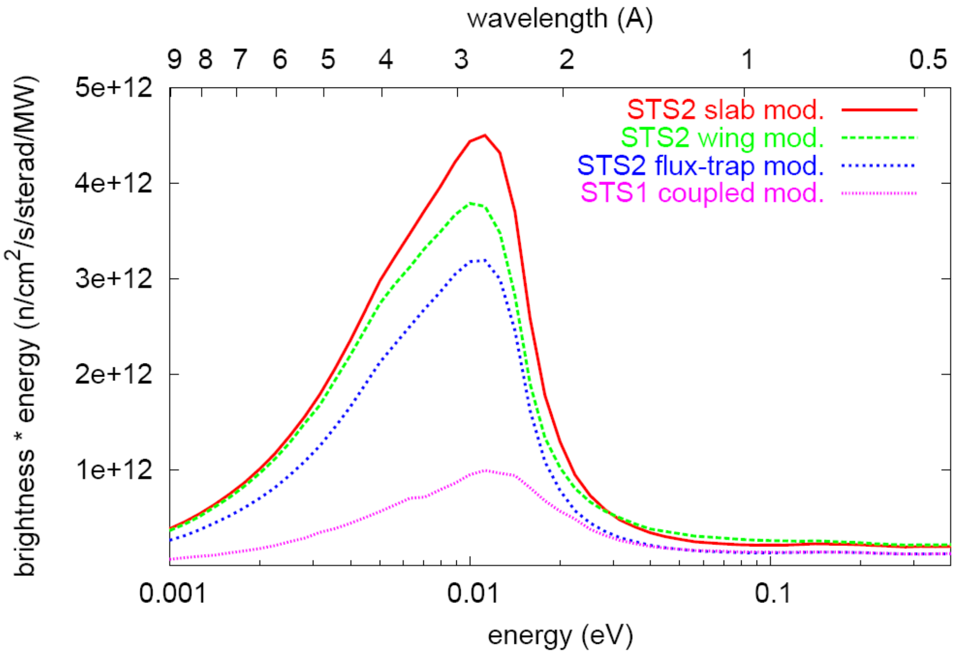

Fig. 3.3. Time-averaged neutron brightness from optimized configurations for slab, volume wing, flux-trap, and the existing SNS target station normalized to 1 MW beam power.

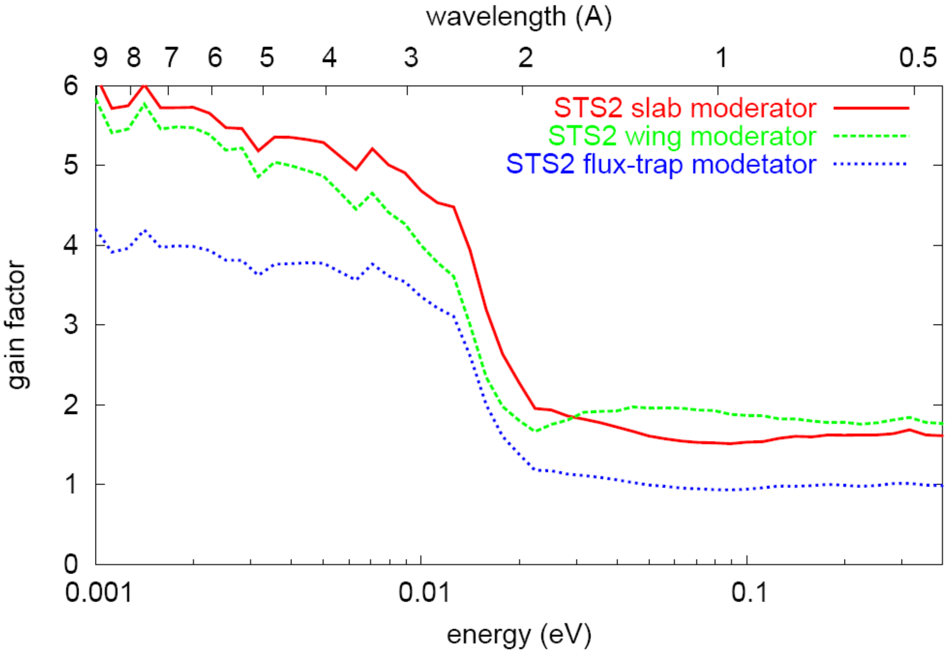

Fig. 3.4. Increase in the neutron brightness for the studied slab, volume wing, and flux trap moderator configurations for the STS relative to the FTS.

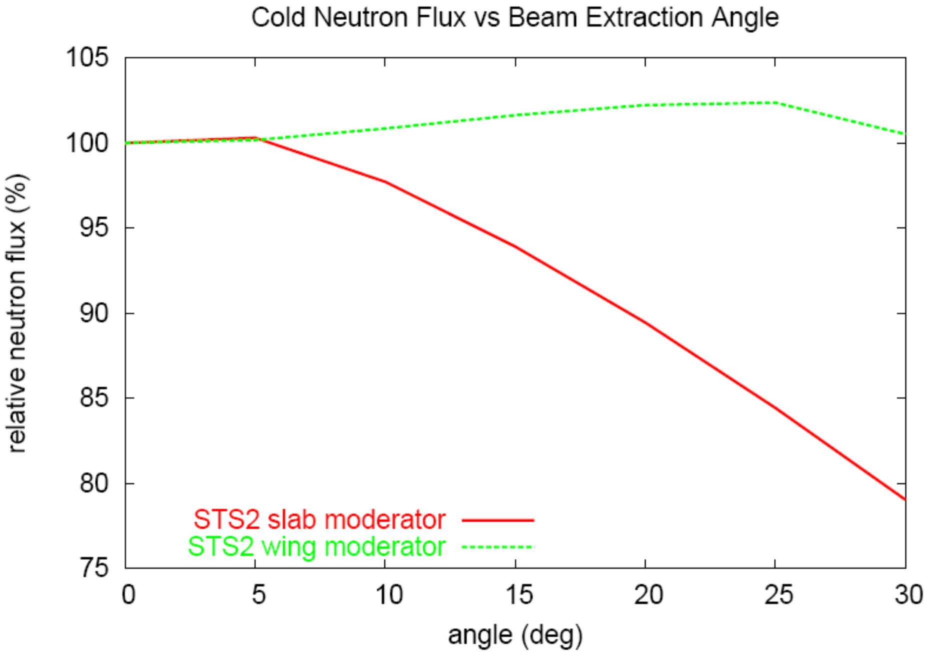

Fig. 3.5. Neutron brightness extracted relative to the brightness at normal incidence as a function of beam extraction angle.

3.4.3 Target Design Concept

A mercury target similar to the first SNS target is the reference design. The principal reason for this selection was the desire to be able to upgrade in the future from 1 to 3 MW. The extrapolation of the mercury target design to 3 MW is considered a low risk, particularly for long-pulse operation. Much of the technology development and safety studies done for the first target station will be applicable to the new design. Although conventional solid target designs showed some performance advantages at 1 MW, at higher power, the performance advantage would be lost; and designing for the activation and decay heat removal for a solid target was judged to be a significant disadvantage. In addition, changing from a solid water-cooled target system at 1 MW to a mercury system for a power upgrade to 3 MW is not desirable. It probably would require a very long shutdown and greatly complicate the design, since much of the work would have to be done by remote handling.

R&D is planned to confirm that cavitation damage is not an issue for the mercury target with long-pulse operation. Even if cavitation damage were an issue, damage mitigation methods developed for the FTS would be used if needed.

Another target option that will be evaluated by the R&D program is a rotating solid target design with water cooling. This option offers the possibility of improved target neutronic performance and much longer target life. Figure 3.6 shows the STS target, wing moderators, and neutron beamlines inside the shielding.

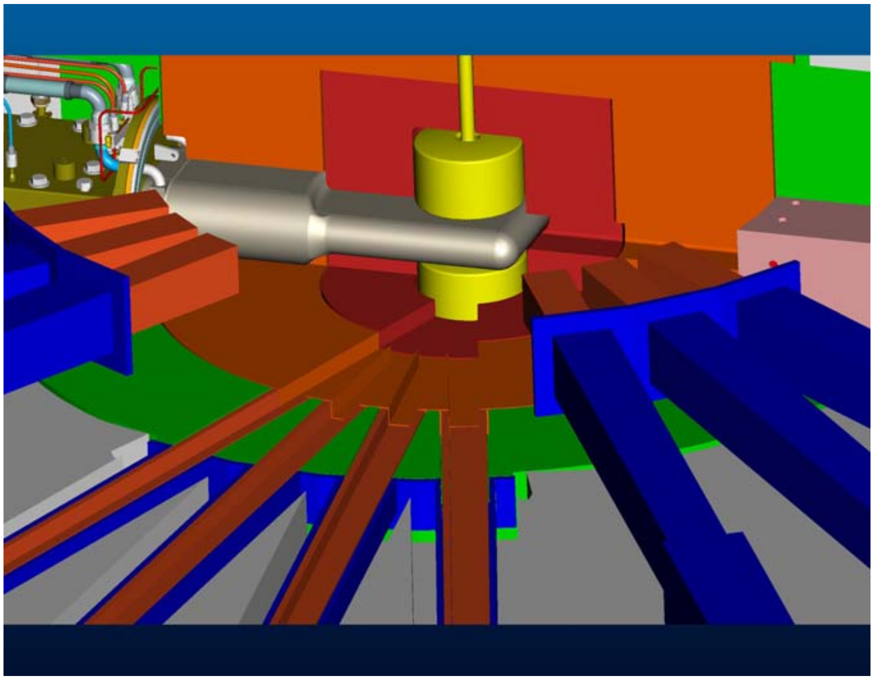

Fig. 3. 6. Cutaway view of target and moderators inside the monolith.

An optimized target vessel design will be developed for the STS, but the overall vessel configuration is expected to be similar to that for the FTS. Long-pulse operation will eliminate the high-pressure pulses developed by short-pulse operation and reduce stresses in the shell.

The mercury process loop and target carriage systems will incorporate the experience gained from the first target station. One change will be the use of magnetic-drive pumps. This technology has advanced since the FTS mercury loop was designed. Figure 3.7 is a prototype of a permanent magnet drive pump developed at the Institute of Physics of the University of Latvia for the ESS program [3.8]. A permanent-magnet-drive type of mercury pump is also currently being developed by the Japanese pulsed source facility (J-PARC) project for its mercury system. This type of pump is expected to be simpler and have fewer problems than the mechanical-drive pump currently being used in the FTS. The additional space in the TSB will allow the use of two pumps to provide redundancy.

3.4.4 Cryogenic Moderator System

The cryogenic moderator system will include a pair of coupled, supercritical hydrogen moderators with the associated hydrogen process loop and a helium refrigeration system. The moderators will be cylindrical Al6061 pressure vessels with inner diameters of 220 mm and a height of approximately 120 mm. The moderators and inner reflector plug (IRP) will be designed for operation at up to 2 MW, which was the design power level for the moderators and reflector plug for the first target station. While the initial operation will be planned for 1 MW, the design will allow for higher power upgrades during the expected 6 to 10 MW-year life of the IRP. The hydrogen loop design will be based on the FTS design with the addition of an ortho-para

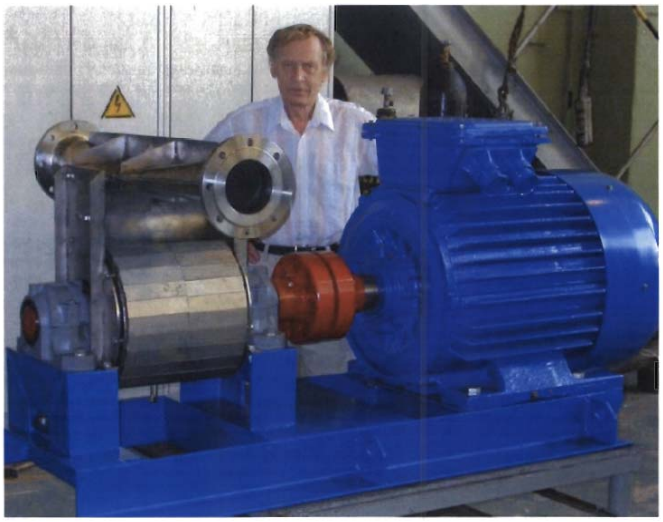

Fig. 3.7. Prototype permanent magnet mercury pump developed for the ESS.

converter and will be designed for the upgrade power level of 3 MW. The helium refrigeration system will be designed with a cold box capable of 2 MW beam operation, but the compressor system will be designed for 1 MW initial operation and will allow for the addition of compressor capacity. A second cold box and compressor capacity would be added above 2 MW to reach 3 MW beam operation. A refrigeration capacity of approximately 10 kW is expected to be needed for 1 MW beam operation.

3.4.5 Monolith Design

The design and construction of the STS monolith has been simplified to reduce the cost and improve the reliability of the target system. Primarily, this can be done because the large, close-in shutters used in the FTS have been replaced with curved beam lines. An immediate advantage results from the relatively simple shielding stack above and below the neutron beamlines. Further, without the large cavities in the shielding required for shutter movement, the shielding stack can be ideally shaped. Thus it requires only the minimum amount of material. As shown in Fig. 3.8, the boundary of the iron shielding approximates a 5.5 m radius above the target instead of extending to the high-bay elevation at the upper corners as required for a shutter-based design. The layout also results in some operational improvements, such as simpler and better-controlled access to the close-in neutron beamline choppers (Fig. 3.9). Preliminary design will include an evaluation of cooling requirements for the bulk shielding for 3 MW operation. It is possible that provision will be needed for air circulation near the central region of the monolith.

3.4.5.1 Core vessel and reflector assemblies

The design for the central region of the monolith will be similar to that for the FTS. The target will be inserted into a vessel that will maintain an inert environment (helium or vacuum) and will contain any mercury releases from the target caused by a major accident such as a seismic event. The two cryogenic moderators and heavy-water-cooled beryllium reflector components will be incorporated into an inner reflector plug designed to be removed vertically

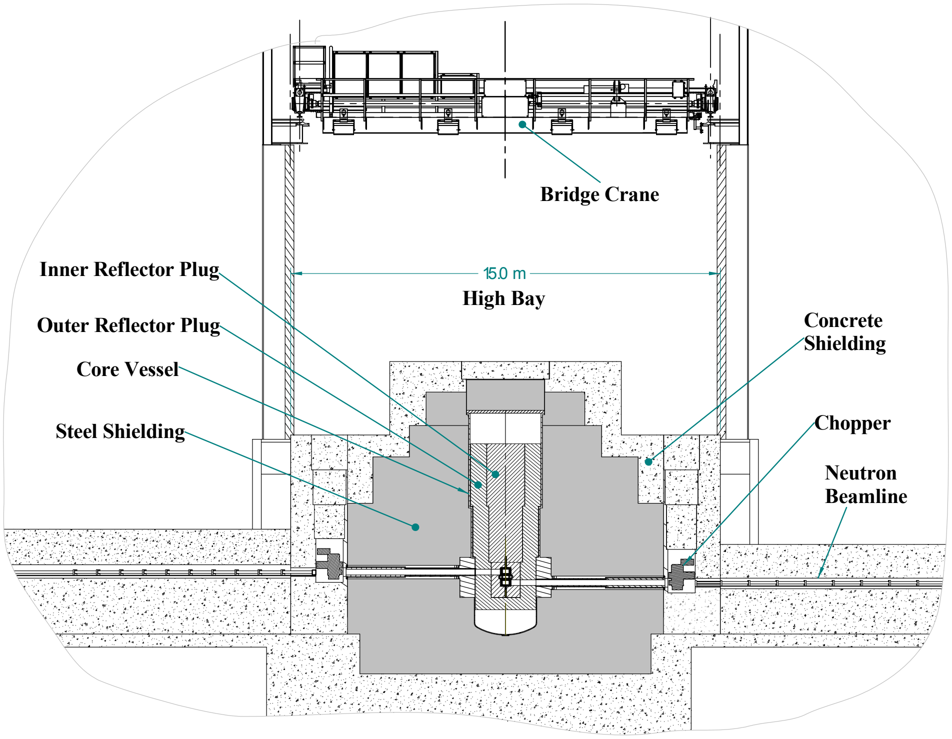

Fig. 3.8. Monolith cross section.

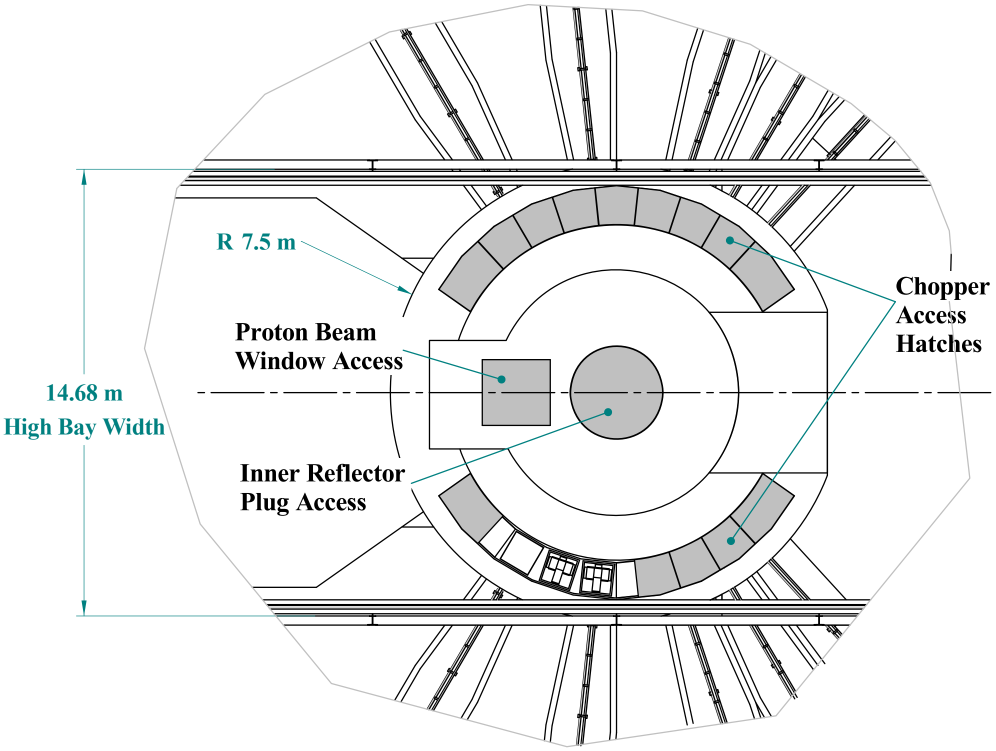

Fig. 3.9. Monolith plan view.

into a shielded cask. Water-cooled iron shielding external to the inner reflector plug will be contained within an outer reflector plug, which will be designed to be replaceable if required, and within the core vessel body near the mid-plane. The proton beam window assembly, similar to that for the FTS,will be located approximately 2 m upstream of the target and will seal to the core vessel on a port extension.

3.4.5.2 Neutron beam lines and choppers

Curved neutron beam lines to limit direct viewing of the target/moderator area will be contained in core vessel port extensions. The port extensions will be permanently mounted to the vessel after the installation of the lower-level iron and concrete shielding. A precision-machined alignment plate will be used to accurately place the extensions. A small gap between the extension and the alignment plate will both protect the extensions and allow for adjustments as the system shifts and settles during the remaining installation process. Neutron guides will be installed in the port extensions between the choppers and a radius of about 1 m. Choppers will be located just outside the iron shielding boundary, centered at about 6.5 m from the target as shown in Figs. 3.8 and 3.9. The choppers will be located in pits cast into the outer shielding layer, where they will be vertically accessible for maintenance and replacement.

3.4.5.3 Beam line and chopper remote handling

Neutron beam guide replacement will be performed with a horizontal extraction and insertion machine in a manner proven in other spallation facilities. Shielding will make this device fairly bulky; therefore, it will be configured for handling with the high bay and instrument floor overhead bridge cranes. Placement of the machine will require the removal of one or more choppers and several meters of neutron beam line. This job is difficult but will only need to performed infrequently.

The first innermost choppers will be changed directly into the high bay with shielded, bottom-loading containers. This approach is efficient and ensures that the activated assemblies are handled entirely within a controlled environment. Downstream choppers and other beam guide apparatus will be handled inside the instrument area of the target building. These units are not expected to be significantly activated and therefore will not require as many shielding or remote handling features.

Neutron beam line shielding and assemblies beyond the 7.5 m boundary will generally be the responsibility of the individual beamline design teams. However, a shielded bunker extending out for several meters will be considered as a means to reduce cost and simplify access to the beamlines. Such a bunker could have handling and access advantages and will be fully assessed as part of the concept optimization program.

3.4.5.4 Shielding

This design using curved neutron beam tubes projecting horizontally from the core vessel allows for extensive use of relatively inexpensive scrap steel for the shielding, in the form of stacked, interleaved blocks. This arrangement eliminates radiation shine paths and provides an efficient and compact monolith. With a fixed horizontal plan reserved for the neutron beam guides, the volume above and below will be filled with crude blocks fitted with metal shims and grout. The poured concrete outer shield can also be efficiently formed around chopper cavities, building structure, and the proton beam window and core vessel access hatches. The horizontally layered build-up of shielding will allow for the use of efficient and safe construction techniques.

3.4.6 Target Service Bay

The proposed layout of the second TSB is closely based on the successful FTS configuration. Thus the proposed system will use similar process and maintenance equipment with lessons-learned and technology improvements added. For example, the length will be roughly the same; however, the width of the cell has been increased to better accommodate spent target handling and sampling. Significant features of the cell will be a stainless steel liner, corbel mounted bridges, a personnel-accessible maintenance cell at the back of the main cell, and several window work stations designed for specific high-intensity tasks such as target change-out and sampling.

Utilities for the TSB will consume approximately the same volume as the cell itself. To avoid interference with the instruments and high bay activities, these systems will be located in the basement. They include the primary and secondary off-gas systems, the low-level liquid waste system, and a bottom-loading waste removal hatch. Provision also will be made for temporary storage of spent targets in the floor of the TSB.

3.5 REFERENCE INSTRUMENT SUITE

In order to better assess the full potential of the facility concept defined in the preceding sections, a set of neutron beam instruments has been selected as a reference or “straw man” instrument suite for the STS. The specific instruments selected are based on concepts proposed and evaluated as part of the SNS Second Target Station Instrumentation Workshop [3.4]. In some cases, the instrument designs proposed at the workshop have been modified to fit circumstances (e.g., the maximum beam length that fits on the site is ~130 m) and the performance reevaluated for the new parameters. Performances also have been reevaluated based on the current estimates of the STS source performance. Instruments selected for the STS reference instrument suite are those instruments proposed during the workshop that provide the greatest scientific payoff and benefit the most from the intense cold beams and low operating frequency at the STS. Sections 3.5.1 through 3.5.6 provide details about each of these reference suite instruments, and their basic parameters and approximate performance are summarized and discussed in Sect. 3.5.7.

Several other very good instruments were evaluated at the instrumentation workshop. These would also provide significant scientific payoff, but they are not as well matched to the STS strengths and should instead be considered for construction either at the FTS or at HFIR.

Performance evaluations for the STS instruments in this section are based on simple, high-level arguments and are only approximate estimates of the performance gains relative to the FTS. Better estimates await accurate modeling of the details of the instruments optimized for performance at the respective sources. Nevertheless, the estimates made here contain the essential factors and give a good sense of the magnitudes of gains that should be possible with the STS.

3.5.1 SANS

3.5.1.1 High-throughput SANS

3.5.1.1.1 Science drivers

SANS is one of the primary tools for studying structures over multiple length scales ranging from less than a nanometer to 1000 nanometers or more. Such studies play an important role in chemistry, biology, complex fluids, and metallurgy, as well as in understanding some more fundamental phenomena such as vortex lattices in superconductors. Structural studies over multiple length scales extending to nanometer dimensions are important for understanding mesoporous materials and self-assemblies of nanometer-scale building blocks.

SANS plays a particularly important role in the area of "soft matter", which includes a wide range of molecular materials such as polymers, liquid crystals, micellar solutions, microemulsions and colloidal suspensions, and biological membranes and vesicles. Such materials have a wide range of applications in areas as diverse as structural and packaging materials, foams and adhesives, detergents, cosmetics, paints, food additives, lubricants and fuel additives, and rubber in tires. SANS can be used to study the time-evolution of structures of self-assembled phases, including systems containing natural or synthetic proteins and nucleic acids with lipids and polymers. Knowledge of the structure of biological macromolecules is essential to the understanding of the functions of these macromolecules at the molecular level. Structural measurements using high-intensity SANS with good signal-to-noise capabilities coupled with specific deuteration can provide information about the positions of individual residues on proteins and multicomponent macromolecular structures in solution, and about the protein folding in solution. Similar techniques can also be used to determine the kinetics, stoichiometry, and organization of large macromolecular complexes, and for structural studies of the hydration of macromolecules and the formation of solvation spheres around macromolecules in solution. They can also play an important role in the study of the conformational transformations in biomacromolecules.

To cover the full range of length scales, a suite of different SANS instruments is required. However, a large fraction of the science of interest occurs within the length scale range of about 6 to 6000 Å (10^{-3} Å$^{-1} < Q < 1$ Å^{-1}), which is the range this particular "workhorse" or high-throughput SANS instrument is designed to address and is somewhat better resolution than is provided by the EQSANS instrument at the FTS. This high-throughput SANS is optimized to provide very high data rates, to enable studies of small or dilute samples, and to carry out kinetic studies to probe the time dependence of changes occurring over this length scale.

3.5.1.1.2 Instrument design and performance

The wavelength resolution required for this instrument is $\delta\lambda/\lambda < 5\%$. This wavelength resolution is proportional to $\delta t/t$ (where *t* is the TOF and δt is the source pulse width). A cold coupled moderator on a short-proton-pulse spallation source produces a neutron pulse a few hundred microseconds wide. This may be extended to approximately one millisecond or more for a long pulsed source. The wavelength resolution due to the neutron pulse width is shown for a 1 ms wide pulse (the baseline case) in long-proton-pulse mode in Fig. 3.10. It is recognized that for reactor-based SANS, $\delta\lambda/\lambda$ (which is also the bandwidth $\Delta\lambda/\lambda$) typically varies from 5 to 30%.

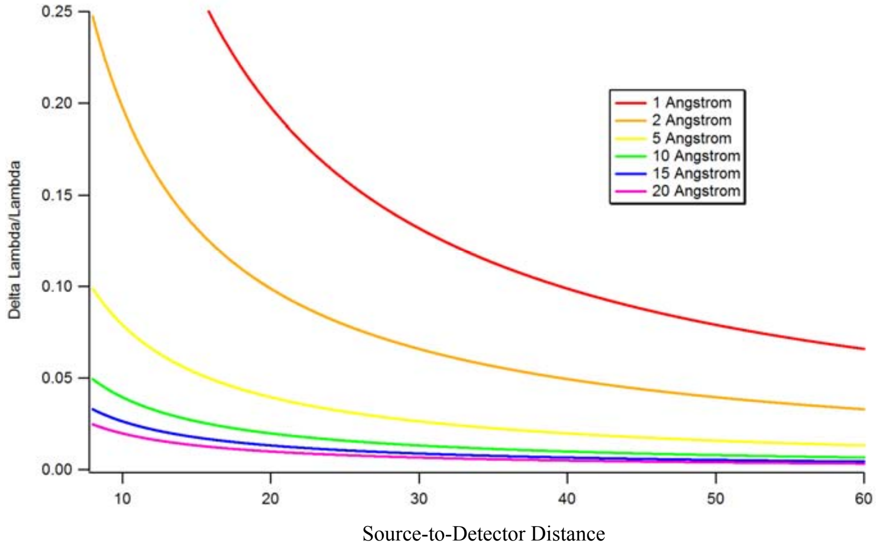

Fig. 3.10. The resolution of a SANS instrument, δλ/λ, as a function of instrument length and wavelength. The pulse width is assumed to be 1 ms.

At this stage of optimization for the high-throughput SANS concept, we have considered a traditional, movable detector SANS with a 1 m^2 detector with 5 mm^2 pixels. We assume a standard, symmetric geometry with a 1 cm diameter sample aperture. The TOF is tunable to select wavelengths between a minimum of 2 Å and a maximum of 15 Å, with the bandwidth determined by TOF (Fig. 3.11). There is assumed to be an exclusion zone of 8 m from the source in which no collimation elements or choppers are placed. Figure 3.12 shows schematically what this instrument would look like.

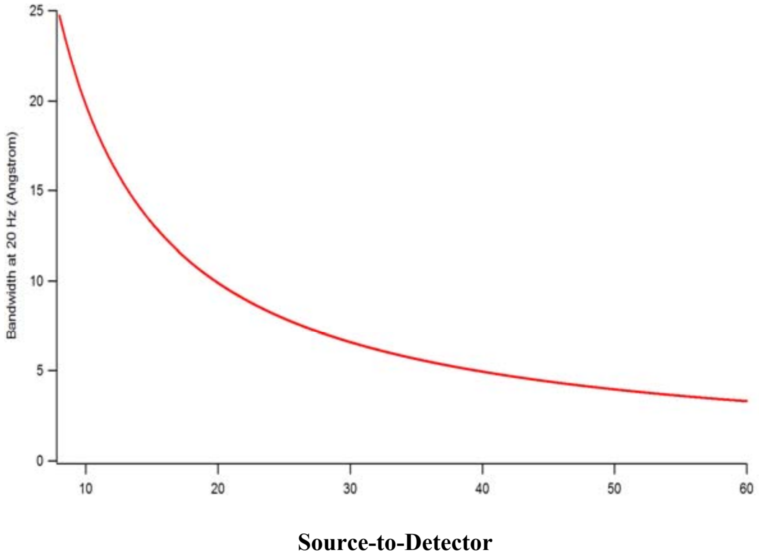

Fig. 3.11. Bandwidth vs the moderator-to-detector distance for the baseline 20 Hz pulsed source.

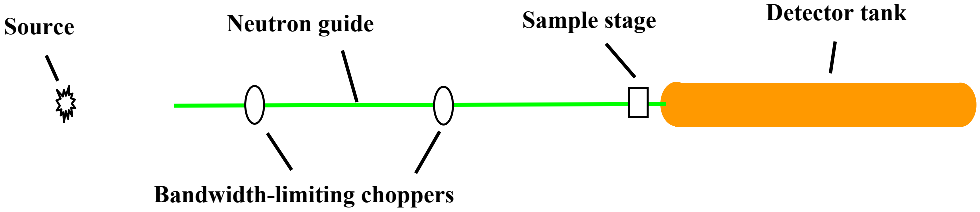

Fig. 3.12. Schematic representation of the high-throughput SANS.

Table 3.2 lists approximate performance parameters estimated for such an instrument. The gain over the same instrument at the FTS (for the same proton beam power delivered to the target) would be a factor of ~16.5 (factor of 5.5 for source intensity and factor of 3 for larger bandwidth resulting from lower repetition rate).

Table 3.2. Performance characteristics for the high-throughput SANS instrument

L_1 (m)	L_2 (m)	λ_{min} (Å)	λ_{max} (Å)	Q_{min} (Å^{-1})	Q_{max} (Å^{-1})
20	12	9	15	0.0010	0.039
20	6	8	15	0.0021	0.087
20	3	7	15	0.0042	0.20
20	1.5	7	15	0.0084	0.40
20	12	2	8	0.0020	0.17
20	6	2	9	0.0035	0.35
20	3	2	10	0.0063	0.70
20	1.5	2	10	0.013	1.4

L_1 = source-to-sample distance; L_2 = sample-to-detector distance; λ_{min} = minimum wavelength used; λ_{min} = maximum wavelength used; Q = wavevector transfer.

3.5.1.2 Biology SANS

3.5.1.2.1 Science drivers

The characteristics defined for the high-throughput SANS are very well suited for the study of biological structures. However, different sample handling and optimization of the sample area are required, a large demand for biological structural studies is expected, and biological structural studies are expected to be slow, so the STS will have a separate biology SANS. This instrument will be optimized for a wide variety of biological structural studies and will provide the sample environment and support equipment necessary for such studies.

3.5.1.2.2 Instrument design and performance

The main parameters for this instrument will be the same as for the high-throughput SANS, except that the sample area and sample preparation laboratories will be optimized to accommodate a range of biological studies. The instrument will look schematically much as shown in Fig. 3.12, and the gains relative to a similar instrument at the FTS at the same proton beam power will be a factor of ~16.5, as described in Sect. 3.5.1.1.2.

3.5.1.3 High-resolution SANS

3.5.1.3.1 Science drivers

This particular "high-resolution" instrument is optimized to cover a length scale range of about 60 to 60,000 Å (10^{-4} Å^{-1} <Q< 10^{-2} Å^{-1}), which addresses significantly larger length scales than does the high-throughput SANS of Sect. 3.5.1.1. This higher resolution is achieved at the expense of data rate, so this instrument will be less well suited to kinetic measurements. It will thus be complementary to the high-throughput SANS instrument, and both will be required to meet the scientific demands. This high-resolution SANS will be particularly good for studying ordering in colloids, 2-dimensional structure in aligned polymers, strained materials, polymer crystallization, polyelectrolyte structures, viruses, pharmaceuticals, and vortex lattices in superconductors.

3.5.1.3.2 Instrument design and performance

For this instrument, we consider a traditional, symmetric long baseline SANS with focusing. As for the high-throughput SANS, the wavelength resolution required for this instrument is $\delta\lambda/\lambda < 5\%$. We again consider a 1 cm source aperture with the beam focused to 1 cm on the detector. Figure 3.13 shows schematically what this instrument would look like.

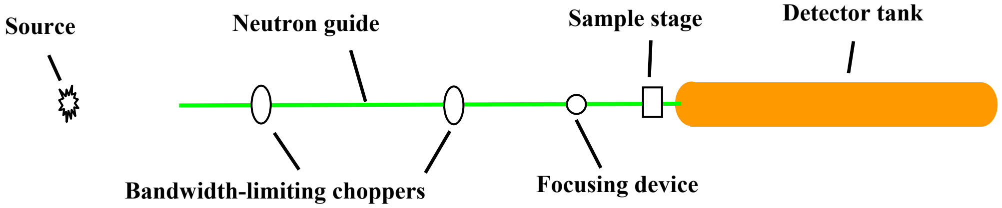

Fig. 3.13. Schematic representation of the high-resolution SANS .

Schematically, this instrument appears very similar to the high-throughput SANS sketched in Fig. 3.12, although the flight-path lengths are somewhat longer for this high-resolution SANS and this instrument has the focusing optics.

Table 3.3 lists approximate performance parameters estimated for such an instrument. Again, the same-instrument gain over the FTS (for the same proton beam power delivered to the target) is about a factor of 16.5.

Table 3.3. Performance characteristics for the high-resolution SANS instrument

L_1 (m)	L_2 (m)	λ_{min} (Å)	λ_{max} (Å)	Q_{min} (Å^{-1})	Q_{max} (Å^{-1})
26	18	16	20	0.00026	0.015
26	12	9.5	14.5	0.00054	0.037
26	6	3	9	0.0017	0.23

L_1 = source-to-sample distance; L_2 = sample-to-detector distance; λ_{min} = minimum wavelength used; λ_{min} = maximum wavelength used; Q = wavevector transfer.

3.5.1.4 Spin-echo SANS

3.5.1.4.1 Science drivers

The spin-echo SANS (SESANS) instrument provides the capability to access still longer length scales than can be reached with the high-resolution SANS. It will be able to span the range from about 50 Å to 100 μm (10^{-5} Å^{-1} <Q< 10^{-2} Å^{-1}). With this range, it will provide capabilities that extend but overlap significantly with those of the high-resolution SANS, but it will also have quite different signal-to-noise characteristics from the high-resolution SANS. Because it uses a spin-echo technique, it may also present some difficulties in working with depolarizing samples (e.g., magnetic samples, samples with large amounts of hydrogen). Thus, again, both instruments will be needed to provide the full range of capabilities. SESANS will be particularly good for the study of composites, agglomerates, powders and colloids, phase transitions and nucleation in ferrites and austenites, geology, transport in soil, carbon sequestration, environmental science, nucleation of bubbles, and large-scale artificial structures.

3.5.1.4.2 Instrument design and performance

The SESANS technique [3.9] uses the Larmor precession of the spin of the neutron to compare the angle of the neutron before and after it is scattered by the sample. Figure 3.14 shows schematically how this process works.

This arrangement consists in principle of two precession regions with parallel inclination faces. With opposite precession in the two regions, we have the spin-echo mode in which the intensity on the detector is proportional to the polarization of the beam after the sample. As indicated in the figure, the polarization is sensitive to small-angle changes of the beam between the two precession regions. This is the normal SESANS mode that enables measurement of the scattering density-density correlation of inhomogeneities. The range of sensitivity is proportional to the square of the wavelength, the magnetic field in the precession regions, the length of the regions, and the inclination angle of the front faces of the regions. Depending on the instrumental details, spin-echo lengths of from 5 nm to 100 μm are achievable.

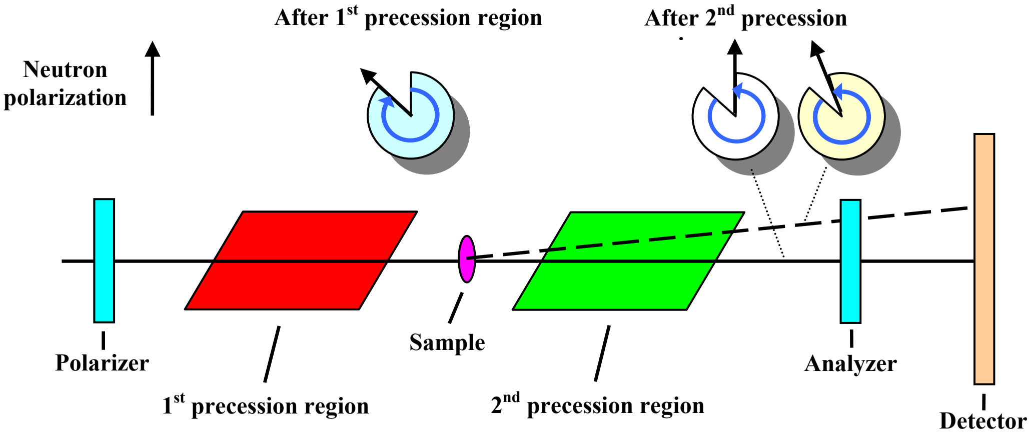

Fig. 3.14. Schematic representation of the SESANS principle

The source-sample distance for this instrument will be ~24 m, and the sample cave will provide a flexible arrangement to allow different configurations of the spin-echo and other optics both before and after the sample. As for the other SANS instruments, this instrument at the STS will have a factor of ~16.5 higher data rate than would a comparable instrument at the FTS at the same proton beam power.

3.5.2 Reflectometry

3.5.2.1 High-intensity horizontal-surface reflectometer

3.5.2.1.1 Science drivers

Reflectometers probe boundaries between materials and measure nuclear and magnetic density profiles perpendicular to planar interfaces. Reflectometry also gives information about interfacial roughness and has provided information about the in-plane structure of thin films. Given the fundamental importance of interfacial phenomena in biology, chemistry, polymer science, structural materials, and artificially layered magnetic systems, reflectometry is expected to continue to play a crucial role in deepening our understanding of important scientific issues, many of which are technologically important. Neutron reflectometers are uniquely sensitive to vector magnetization and to isotopic substitution, most notably the use of deuterium (^{2}H) for contrast enhancement. The following is a partial list of past, current, and future fields of interest.

- Phase separation in polymer and copolymer films
- Inorganic templating at air/water interfaces
- Complex fluids under flow
- Vesicles and gels
- Reaction kinetics at surfaces
- Surfactants at interfaces
- Interfacial structure in drug delivery systems
- Membranes and their intermolecular interaction
- Protein adsorption to surfaces and membranes
- The effect of surfaces on critical phenomena in fluid systems
- Biocompatibility and sensors
- Multilayer materials (e.g., giant magnetoresistance [GMR]) for magnetic recording
- Depth-dependent domain imaging
- In-situ characterization of molecular beam epitaxy (MBE)-grown layers
- Magnetic monolayers and multilayers
- Superparamagnetic nanoparticles
- Exchange-biased interfaces
- Magnetic tunnel junctions
- Hard/soft magnetic multilayer combinations

A suite of differently-optimized reflectometers will be required at the STS to provide the optimum capabilities for addressing these diverse areas of science.

Sample positioning and alignment is extremely important in reflectivity measurements. Reflectometers are generally built to study either horizontally or vertically mounted samples.

Horizontal sample mounting is necessary to study free-liquid surfaces, while vertical mounting schemes are generally more compatible with standard sample environment equipment, such as superconducting magnets or cryostats. Positioning systems for the STS reflectometers will generally conform to one or another of these schemes.

A high-intensity horizontal-surface reflectometer for the STS is described in this section, and a complementary high-intensity vertical-surface reflectometer for the STS is described in Sect. 3.5.2.2. This horizontal-surface instrument will be optimized for the study of liquids, membranes, and other interfaces that must be horizontal or nearly horizontal for such measurements. These categories include a significant fraction of the scientific areas listed above. Because of the intense cold beams and low repetition rate available at the STS, along with a number of the other design features discussed in the following paragraphs, this instrument will be able to extend kinetic studies of phenomena occurring at such interfaces to explore processes with much shorter time-constants. These features will also enable the study of much smaller samples that may be required when complex specialized sample environments are used. Furthermore, this instrument will be configured to permit simultaneous complementary measurements such as X-ray reflectivity or Brewster-angle microscopy.

3.5.2.1.2 Instrument design and performance

The various reflectometers at the STS will have a significant commonality in instrument configuration, particularly the neutron guides, choppers, and detectors. They will all use multi-channel curved guides to eliminate direct line-of-sight and deliver almost all of the available flux at the 2.5 Å peak of the coupled H_2 moderator in a 20–40 m moderator-detector distance. Specularly reflected neutron beams are generally quite compact, so reflectometer detectors are normally small ($< 20 \times 20$ cm^2), featuring moderate (1 mm 1-dimensional or 1 mm^2 pixel resolution 2-dimensional position-sensitive detectors) or coarse (^{3}He tubes) spatial resolution. The spatially diffuse nature of off-specular reflectivity and grazing-incidence scattering may more profitably be measured using larger fixed banks of detectors.

Figure 3.15 shows a schematic representation of the high-intensity horizontal surface reflectometer. In addition to the neutron guide system discussed above, the incident beam will have bandwidth-limiting choppers to enable precise control of the range of wavelengths reaching the detector. It will also include a pulse-shaping chopper to control the neutron pulse width or to cut off the tail of the pulse to improve background when necessary. The secondary portion of this instrument—including the final front-end optics, the sample region, and the detector arm and its associated motions—will be designed to be very flexible and reconfigurable. These features allow this instrument to accommodate a variety of incident beam final optics and a variety of different types of sample environments. The low repetition rate of the STS still provides an adequate wavelength bandwidth with this instrument at a source-to-sample distance of 30 m; at this distance, there will be more floor space between neighboring instruments, permitting this section of the reflectometer to be housed in “spacious” quarters (by reflectometer standards). This will provide the space to accommodate exotic sample environments or to allow extensive incident beamline modification and to carry out concurrent complementary measurements. As shown in Fig. 3.15, the detector arm can swing through a range of angles, permitting the study of diffraction from multilayer systems as well as covering the full range of reflection angles.

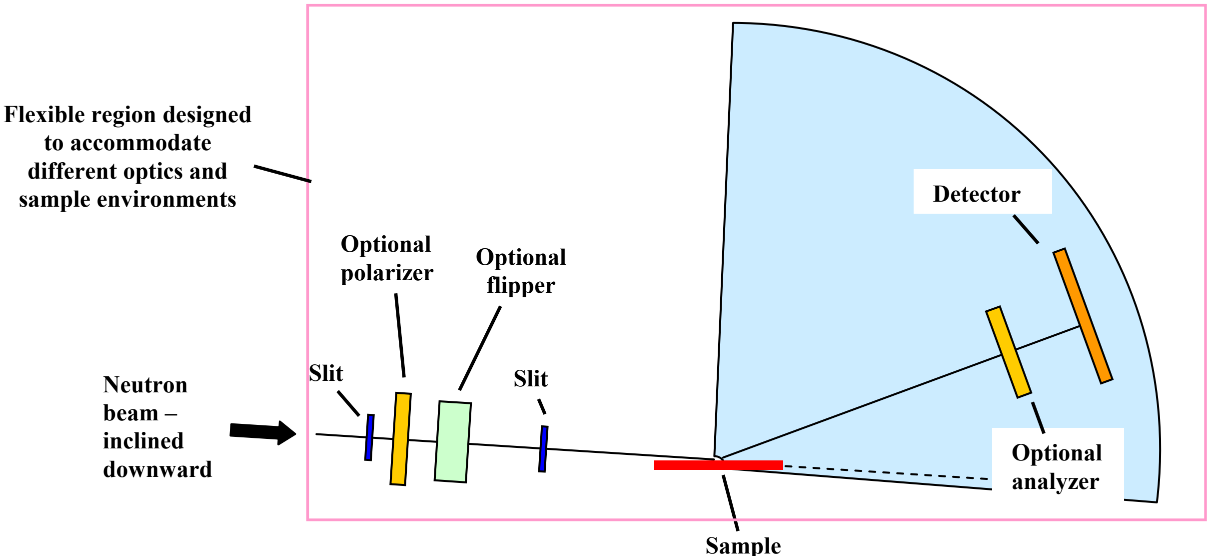

Fig. 3.15. Schematic elevation view of the high-intensity horizontal-surface reflectometer. The scattered beam measurement arm swings around through the shaded arc shown. The incident beam has a neutron guide and bandwidth choppers (and, optionally, a pulse-shaping chopper) that are not shown in this view.

This instrument, at a short-proton-pulse version of the STS, will provide a factor of ~11 higher data rate than would a comparable instrument at the FTS. A large part of that gain (a factor of ~5.5, assuming equal proton power is delivered to both targets) comes from the increased moderator brightness at the STS, whereas an additional smaller factor (~2) derives from the reduced source frequency (not all the bandwidth is equally useful, as discussed by Fitzsimmons [3.10]). The wavelength resolution with either the short-proton-pulse or the long-proton-pulse option is adequate at this distance for most experiments [3.10]. For most cases, therefore, the overall gain factor is essentially the same for a long-proton-pulse option with equal proton beam power and equal frequency. In either case, the longer flight path permitted by the lower repetition rate at the STS should also lower the instrument background.

3.5.2.2 High-intensity vertical-surface reflectometer

3.5.2.2.1 Science drivers

A high-intensity vertical-surface reflectometer for the STS is described in this section. This instrument is similar to the complementary high-intensity horizontal-surface reflectometer for the STS described in Sect. 3.5.2.1; but, as the name implies, this instrument is designed with a vertical rather than horizontal sample geometry. The high-intensity vertical-surface reflectometer will be optimized for the study of samples and sample environments that work best in the vertical-surface geometry. Examples include a number of different types of studies involving magnetism in thin-film samples with the high magnetic field supplied by a cryomagnet. The vertical sample geometry also permits coverage of a full range of scattering angles in the reflection plane, making this geometry ideal for diffraction measurements to study details of inter-planar spacings in multilayer systems.

A significant fraction of the experiments on this instrument will involve the use of polarized neutrons. Full neutron polarization analysis is not always used in neutron reflectometry experiments. Often it is sufficient to polarize the incident neutron beam and to measure the specular reflectivity for incident neutrons polarized both parallel and antiparallel to a (usually saturating) magnetic field applied to the sample. More information can be obtained by analyzing both the Q-dependence and the neutron spin dependence of diffusely scattered neutrons. In particular, this technique has been used to obtain unique information about helical and fan-like magnetic structures in layered systems. Until now, however, these types of measurements have involved measuring only one component of the spin of the reflected neutrons. Even more information about the vector magnetization within a layered structure could be obtained by measuring the full tensor dependence of the polarized neutron scattering cross section. In this type of measurement, often known as generalized polarization analysis or spherical neutron polarimetry, the direction of the polarization of incident neutrons is controlled and the polarization direction of the scattered neutrons is accurately determined. Experiments at Institut Laue-Langevin (ILL) (the only place where this technique has been extensively developed) have shown that, with bulk samples, exquisite information about magnetic structure can be obtained. The STS high-intensity vertical-surface reflectometer will provide an option for applying the same technique to reflectometry, where it is expected to make available the same improvement in the quality of information.

This instrument (using the spherical neutron polarimetry option when appropriate) will provide highly detailed additional information as necessary to allow researchers to address forefront scientific problems in magnetism and in magnetic systems and devices, including multilayer materials (e.g., GMR) for magnetic recording, depth-dependent domain imaging, in-situ characterization of MBE-grown layers, magnetic monolayers and multilayers, superparamagnetic nanoparticles, exchange-biased interfaces, magnetic tunnel junctions, and hard/soft magnetic multilayer combinations.

Because of the intense cold beams and low repetition rate available at the STS, along with a number of the other design features discussed below, this instrument will be able to extend kinetic studies of phenomena occurring at such interfaces to much shorter time-constant phenomena. These features will also enable the study of much smaller samples, which may be required when complex specialized sample environments are used. This instrument will also be configured to permit simultaneous complementary measurements such as X-ray reflectivity, Brewster-angle microscopy, or magneto-optic Kerr effect (MOKE).

3.5.2.2.2 Instrument design and performance

Figure 3.16 shows a schematic representation of the high-intensity vertical-surface reflectometer. This instrument will have a neutron guide system and a suite of incident beam choppers similar to those discussed in Sect. 3.5.2.1.2. The secondary portion of this instrument—including the final front-end optics, the sample region, and the detector arm and its associated motions—will be designed to be very flexible and reconfigurable. Thus this instrument will be able to accommodate a variety of incident beam final optics and a variety of different types of sample environments, all of which require the sample surface to be vertical or near vertical. The low repetition rate of the STS still provides an adequate wavelength bandwidth with this instrument at a source-to-sample distance of 30 m; at this distance the floor space between neighboring instruments will provide the space to accommodate exotic sample environments or to allow extensive incident beamline modification and to carry out complementary measurements. The vertical-surface geometry allows the detector arm to swing through a large range of angles,

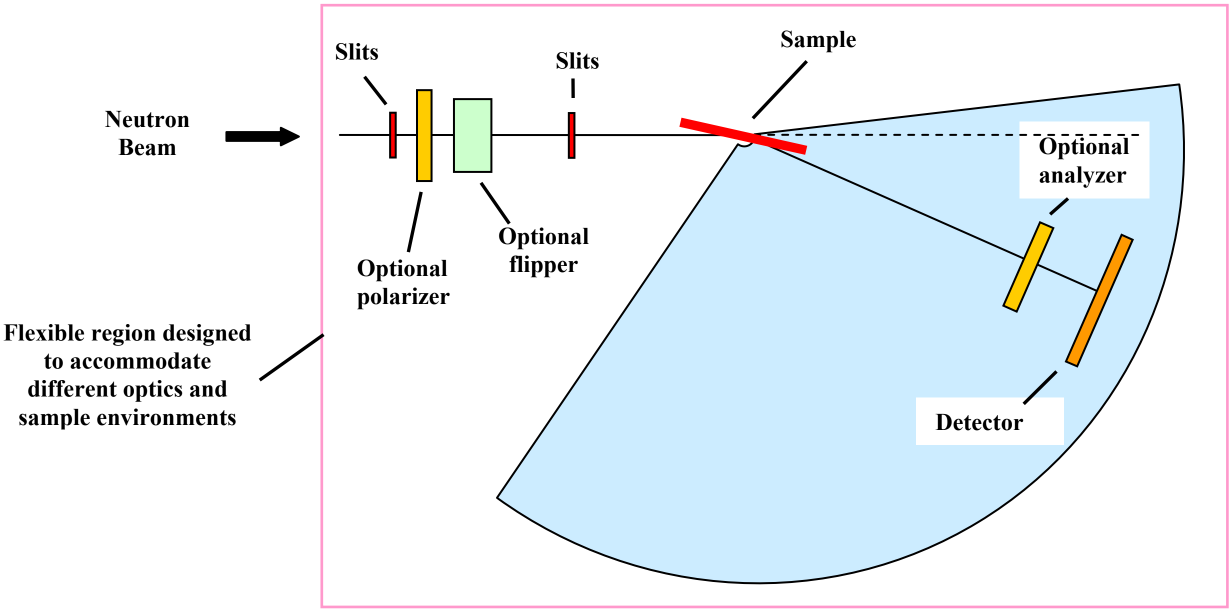

Fig. 3.16. Schematic plan view of the high-intensity vertical-surface reflectometer. The scattered beam measurement arm swings around through a full range of in-plane scattering angles (shown schematically by the shaded arc) or, alternatively, this full arc can be covered with detectors. The incident beam has a neutron guide and bandwidth choppers (and, optionally, a pulse-shaping chopper) that are not shown in this view.

making this instrument exceptionally good for the use of diffraction to probe details of the inter-planar separations.

This high-intensity vertical-surface reflectometer at a short-proton-pulse version of the STS will provide a factor of ~11 higher data rate than would a comparable instrument at the FTS. As discussed in Sect. 3.5.2.1.2, a large part of that gain (a factor of ~5.5, assuming equal proton power is delivered to both targets) comes from the increased moderator brightness at the STS; an additional smaller factor (~2) derives from the reduced source frequency. Also, for most experiments, this overall factor would be about the same for a long-proton-pulse option with equal proton beam power and equal frequency, as discussed in Sect. 3.5.2.1.2. In either case, the longer flight path permitted by the lower repetition rate at the STS also should also lower the instrument background.

This instrument will be designed for standard polarized beam operation and analysis, with the option for generalized polarization analysis for problems that warrant such in-depth studies. It will follow traditional design principles for a polarization neutron reflectometer and will also be equipped with devices (like the ILL cryopad [3.11]) to manipulate the polarization of neutrons incident on and scattered from the sample. It will be designed so that these devices can be mounted as needed; otherwise, it will function in the traditional reflectometer manner, with or without polarization, already implemented at the FTS.

3.5.2.3 Grazing-incidence diffraction and grazing-incidence SANS

3.5.2.3.1 Science drivers

In grazing-incidence diffraction (GID) and grazing-incidence SANS (GISANS), the incoming neutrons strike the interface at an angle smaller than the critical angle. The resulting evanescent wave scattering occurs in an interfacial region with a thickness determined by the wavelength of the neutrons, the contrast (difference in refractive index of the two media) and the angle. The intensity of the wave decays exponentially normal to the interface. Scattering by the evanescent wave is very weak.

GID is used to measure short-range lateral structure (length scales of a few tenths of a nanometer) within the layer(s). In particular, if the top layer is organized, then 2-dimensional Bragg reflections can be observed in the direction normal to the reflecting plane. In GID experiments, the incident beam wavevector k_i is kept below the critical angle, creating an evanescent wave with finite penetration depth into the bulk of the sample and thus enhancing signals from the surface. An ordered 2-dimensional system gives rise to rod-like Bragg reflections along the z-axis (normal to the surface) that contain information on the scattering density of the ordered objects. The total cross section for scattering from a 2-dimensional system is in general very small.

GISANS measures large length scales (~5 to 100 nm). Figure 3.17 shows the scattering geometry. As in GID, the total cross section for scattering is very small. Until now, GID and GISANS experiments have mostly been done on standard reflectometers or SANS instruments. However, the high intensity of the cold neutron beams at the STS will make it possible to access these types of information from a much wider variety of systems and is expected to increase demand for such measurements. Even with the STS, the signals in GID and GISANS will be very weak, and it will be important to have a separate instrument dedicated to and optimized for these types of studies. This instrument will allow researchers to address forefront scientific problems in soft-matter systems, including aspects of phase separation in polymer and copolymer films, in-plane structures occurring during inorganic templating at air/water interfaces or within complex fluids under flow, in-plane structures of vesicles and gels, interfacial structure in drug delivery systems, and structural changes resulting from the interactions of macromolecules with membranes. Areas in hard-matter systems where these techniques can be particularly important include depth-dependent imaging of magnetic domains, in-situ characterization of MBE-grown layers, characterization of magnetic monolayers and multilayers, exchange-biased interfaces, magnetic tunnel junctions, and hard/soft magnetic multilayer combinations.

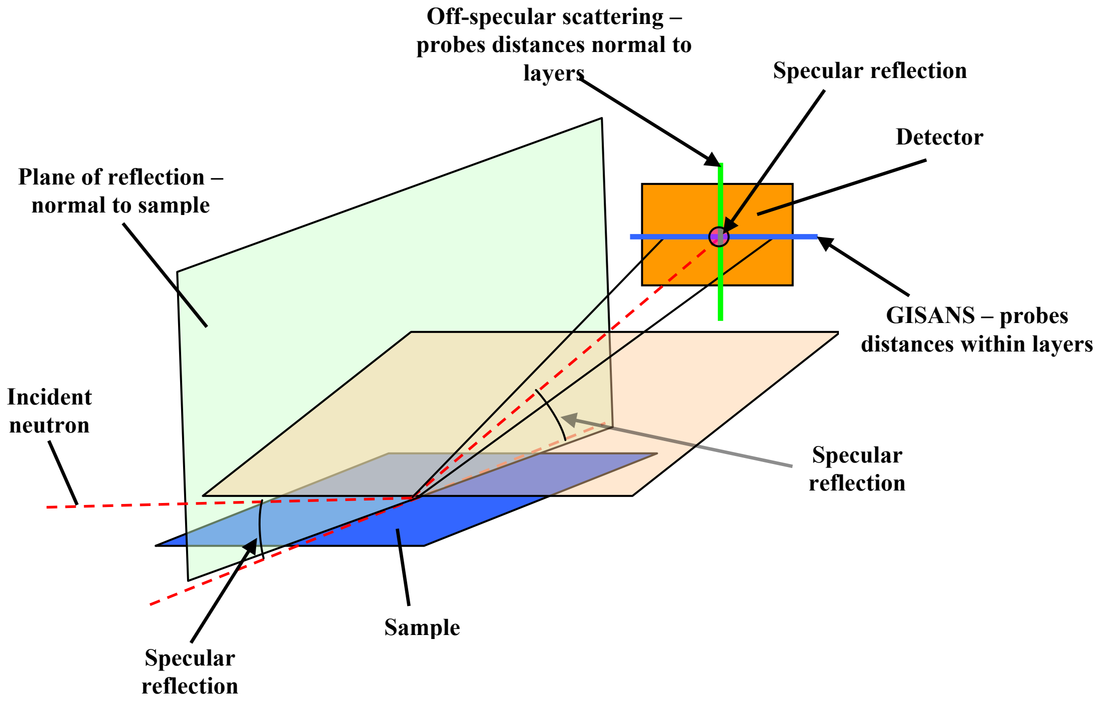

Fig. 3.17. Schematic geometry for grazing-incidence SANS.

3.5.2.3.2 Instrument design and performance

Figure 3.18 provides a schematic representation of an instrument optimized for GID and GISANS at the STS. In order to enhance the intensity on the sample, this instrument will have a converging beam geometry perpendicular to the specular reflection plane. Because many of the scientific problems involve liquids or membranes, this instrument will have a horizontal-sample geometry. The source-sample distance will be 30 m to provide ample room for and access to the focusing optics. In addition to the specialized focusing optics, this instrument will have a wide horizontal sample and a variable-length sample-detector flight path with a maximum length of ~5 m, chosen to provide $Q_{min} = 0.002$ Å^{-1} at 4 Å with a 3 mm beam. The area-detector resolution will be 1 mm vertical and 3–5 mm horizontal and will be 20 cm high × 100 cm wide. It will be able to swing through a horizontal arc to cover scattering angles of up to ~10° for GID.

Like the other reflectometers, this instrument will also have a factor of ~11 higher data rate at the STS than if it were built at the FTS (factor of ~5.5 from source intensity and ~2 from the lower repetition rate). The source-sample distance can be longer at the STS because of the lower repetition rate, and this will lead to a lower background and thus an improvement in signal-to-noise ratio. This improved signal-to-noise ratio will be particularly important because of the weak signals in GID and GISANS and will result in a further significant enhancement in the performance of this instrument compared with a similar instrument at the FTS.

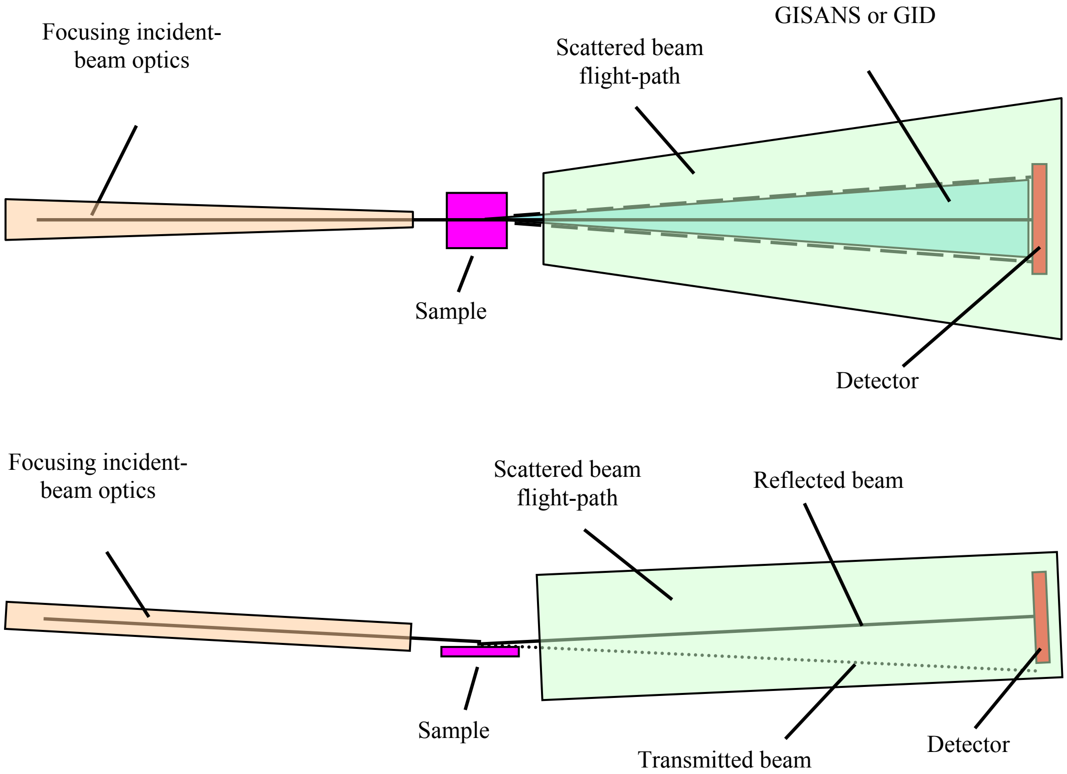

Fig. 3.18. Schematic views of the GID and GISANS instrument. The upper figure shows a plan view and the lower figure an elevation view. The detector translates parallel to the reflected beam and normal to the plane of reflection. The sample surface is horizontal. The incident beam has a neutron guide and bandwidth choppers (and optionally, a pulse-shaping chopper) that are not shown in this view.

3.5.2.4 Spin-echo resolved grazing incidence spectrometer

3.5.2.4.1 Science drivers

Although neutron specular reflectometry has been very successfully employed to probe layered structures, it has been less often used to probe the in-plane structures of thin films and membranes, essentially because the scattering from such low-volume systems is very weak. This problem is exacerbated by the fact that the typical sizes of interesting structures (1–100 nm) require well-collimated neutron beams. To overcome this problem, the technique of spin-echo-resolved grazing incidence scattering (SERGIS) is being developed [3.12]. In SERGIS, scattering angles of a broadly divergent beam are coded by the Larmor precession of neutron spins in a magnetic field in a variant of the well-known neutron-spin-echo method. This technique has recently been successfully tested by a team of U.S. and European researchers at the ILL.

SERGIS is a technique that measures spatial correlations directly in real space rather than in reciprocal space. The technique yields a measure of the projection of the Patterson correlation function along one direction, chosen in the SERGIS case to be in the plane of the reflecting sample. Correlation lengths of up to 300 nm have been measured in the SERGIS geometry in a preliminary experiment at the ILL, whereas distances of up to 20 microns have been measured by the related SESANS technique in bulk samples. There appears to be no inherent reason why such distances should not be achievable in the SERGIS case. By the time the STS is built there are likely to be several possible solutions to the problem of designing suitable spin flippers for pulsed-source applications of SERGIS. Currently, several designs have been proposed and are awaiting thorough testing. It appears likely that the SERGIS and SESANS techniques (Sect. 3.5.1.4) will be developed considerably over the next few years at less powerful neutron sources both in the United States and in Europe.

This instrument will provide measurement capabilities complementary to those of the GID and GISANS Reflectometer discussed in Sect. 3.5.2.3. Forefront scientific problems that can be addressed with this instrument include phase separation in polymer and copolymer films, large-length-scale (from tens of nanometers up to a few microns) in-plane structures occurring during inorganic templating at air/water interfaces or within complex fluids under flow, similar-scale structures of vesicles and gels, interfacial structure in drug delivery systems, and structural changes resulting from the interactions of macromolecules with membranes.

3.5.3.4.2 Instrument design and performance

The SERGIS technique does not require either good neutron wavelength resolution or precise definition of the neutron trajectories with respect to the plane of specular reflection. Within the specular reflection plane, good beam collimation, as provided by the adjustable slits that are traditionally used, is required to separate specular from diffuse scattering on the detector. Thus high index neutron guides can be used to provide broad divergence, at least in one dimension. The only other difference between a SERGIS instrument and a traditional polarized-neutron reflectometer involves the installation of specially designed spin flippers that ensure the Larmor coding of neutron trajectories. Magnetic and magnetizable materials need to be avoided in the construction of the instrument since these can disturb neutron spin precession. The source-sample distance will be ~24 m, to provide low backgrounds. This instrument can use a large wavelength resolution $\delta\lambda/\lambda$ (up to ~0.1). Figure 3.19 shows schematic plan and elevation views of the SERGIS instrument.

Variable-wavelength flippers and beam paths (2 m before and after the sample) are needed for the Larmor precessions. Variable-wavelength polarizers and analyzers are also required. Stray fields must be kept below 0.1 Oe. The space within the reflectometer cave will be designed for flexibility both upstream and downstream from the sample to allow the spin-echo and other components to be configured as needed for particular applications.

As for the other reflectometers, the gains relative to a similar instrument at the FTS will be about a factor of 11.

3.5.2.6 Inelastic reflectometry

The STS will provide enough intensity to enable inelastic neutron scattering measurements of the dynamical processes at surfaces and in thin films and membranes. Two of the neutron resonant spin-echo (NRSE) spectrometers at the STS will be constructed with reflectometer geometry (see Sects. 3.5.4.1 and 3.5.4.2), so those will be the instruments of choice for such measurements.

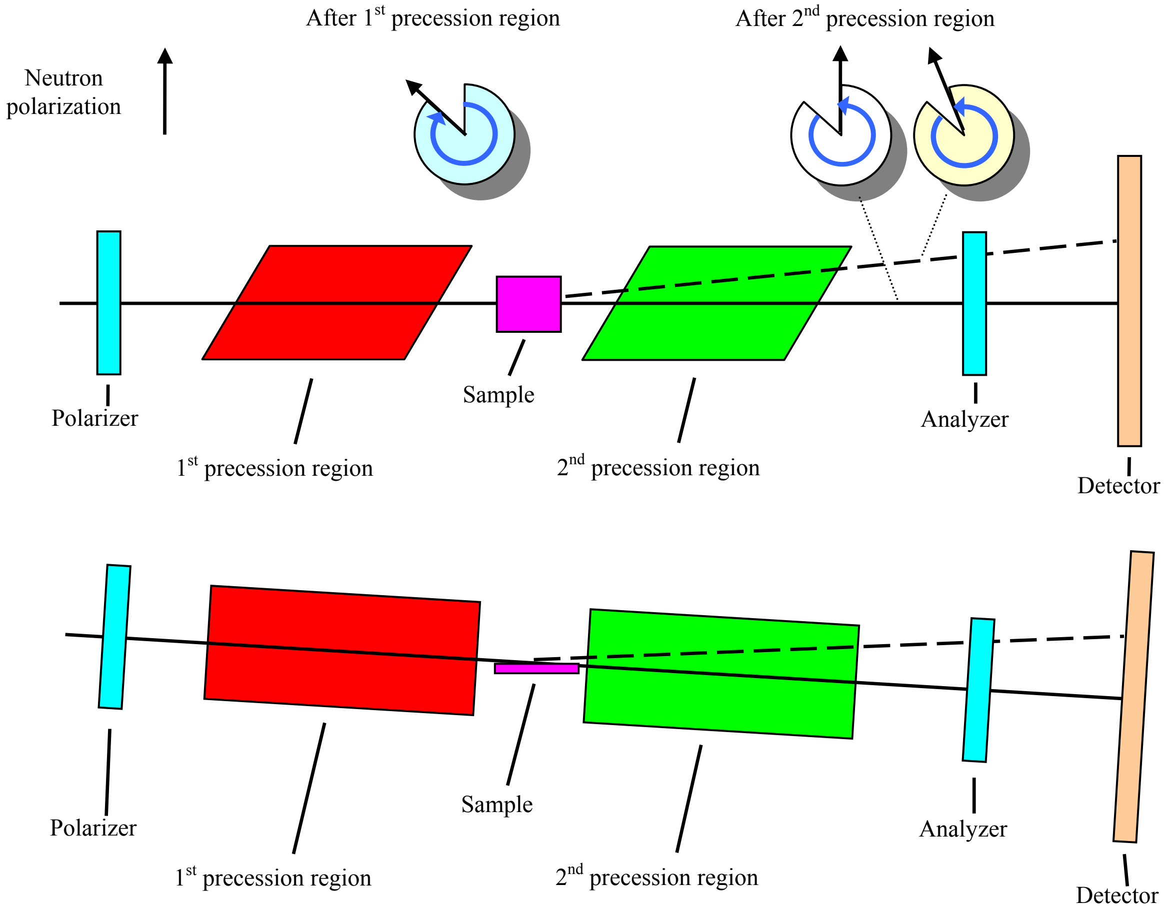

Fig. 3.19. Schematic views of the SERGIS instrument. Horizontal-sample geometry is used in this instrument. The upper figure shows a plan view of the final incident-beam optics, the sample, and the secondary spectrometer. The lower figure shows an elevation view of the same region. The incident beam has a neutron guide and bandwidth choppers that are not shown in these views.

3.5.3 Diffraction

3.5.3.1 High-resolution low-Q neutron diffractometer

3.5.3.1.1 Science drivers

High-resolution neutron diffraction at relatively low Q values, combined with targeted deuteration of specific groups in macromolecules, offers a great deal to the fields of high-resolution structure of membranes, low-resolution structure of membrane proteins, thin polymer composite films, and 2-dimensional devices for biosensors and biotechnology. This instrument will address these problems and many other important problems related to health and biotechnology and to the development of patterned arrays of biomimetic matrices for diagnostic purposes. Furthermore, this instrument will enable the investigation of functional mechanisms of assembly and ordering of antimicrobial peptides in host membranes, methods of assembly and ordering in complex fluids, and self-assembly of nanoparticle arrays in block copolymer matrices for applications in nanotechnology. These systems have length scales ranging from 1 to 600 Å ($10^{-2} < Q < 5$ Å^{-1}), and their investigations require high $\delta\lambda/\lambda$ resolution (~1%) with ΔQ in the range of 0.015 to 0.02 Å^{-1} over the above Q range.

3.5.3.1.2 Instrument design and performance

With a wavelength resolution of $\delta\lambda/\lambda$ ~0.01, an appropriate goniometer, and high-resolution position-sensitive detectors, this instrument will provide medium to high $\delta Q/Q$ resolution.

The 20 to 22 m flight path at the EQSANS instrument at the FTS with an operating wavelength of 5 Å can obtain 1% $\delta\lambda/\lambda$. This wavelength resolution can be achieved at the STS even with the long-proton-pulse option (neutron pulse full width at half maximum [FWHM] ~1000 μs [3.3]) by using 5 Å neutrons on a instrument with a flight path of ~75 m with a resulting bandwidth $\Delta\lambda = 3955/(20 \times 75) = 2.6$ Å. Similar resolution can be achieved on the FTS using 5 Å neutrons with a bandwidth of $\Delta\lambda = 3955/(22{\times}60) = 3.3$ Å. The time-averaged flux at the STS is ~5.5 times that at the FTS (at equal proton power). Hence the overall gain at the STS compared with the EQSANS at the FTS is ~$2.6 \times 5.5/3.0 = 4.8$. For the short-proton-pulse case (neutron pulse FWHM ~300 μs at 5 Å [3.3]), this instrument can be shortened to ~22 m (the same as at the FTS), in which case it will have a bandwidth of ~9 Å and a data rate gain factor relative to EQSANS of ~16.5, assuming all the bandwidth is equally useful). Figure 3.20 shows the STS instrument schematically.

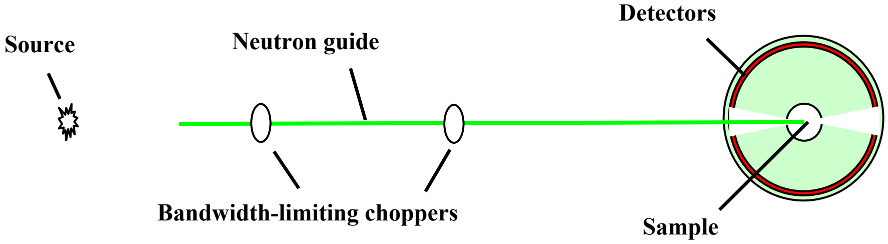

Fig. 3.20. Schematic representation of the high-resolution low-Q neutron diffractometer .

3.5.3.2 High-throughput single-crystal macromolecular diffractometer

3.5.3.2.1 Science drivers

Knowledge of the structure and dynamics of biological macromolecules is essential to an understanding of the functions of these macromolecules at the molecular level. However, at best, the single-crystal samples are very small for these materials. Furthermore, the molecular weight of the protein determines the unit cell volume, which places limits on the molecular sizes that currently can be studied in such weakly scattering crystals. Advancing the forefront with neutron protein crystallography requires extending the instrumentation and the sample preparation capabilities to allow single-crystal structural studies of a much wider range of samples (e.g., high-data-rate/low-background neutron scattering instruments, improved deuteration and crystallization capabilities), thus extending the knowledge of precise locations of functionally important protons to many more macromolecular systems.

A next-generation much-higher-intensity macromolecular neutron diffractometer (MaNDi) is currently under construction at the FTS [3.13]. Given the increased number of protein systems suitable for neutron diffraction studies that has resulted from a reduction in the crystal volume required with such next-generation high intensity instruments, and from advances in protein perdeuteration improving the signal-to-noise ratio, it is reasonable to assume that MaNDi will have a huge over-subscription the instant it is ready for users. A high-throughput MaNDi

(HiMaNDi) at the STS will be complementary to MaNDi and will be optimized to provide much higher throughput for unit cell lengths of less than 100 Å, alleviating the expected burden that will be placed on MaNDi from the biological macromolecular community. Forty percent of the structures deposited into the protein data bank have all unit cell lengths of less than 100 Å, whereas 62% (25861) have all unit cell lengths of less than 150 Å. Perhaps more important, these higher data rates will permit the use of even smaller, weaker-diffracting protein crystals of less than 0.1 mm in volume for study. This development will make the study of many more protein systems feasible using neutron diffraction.

3.5.3.2.2 Instrument design and performance

MaNDi is situated on a decoupled and poisoned hydrogen moderator at the FTS and is optimized to achieve 1.5 Å resolution from crystals 0.2–1 mm^3 with lattice dimensions of up to 150 Å. HiMaNDi will be located on a 130 m incident beam line at the STS, where coupled hydrogen moderators will produce a time-averaged neutron beam intensity a factor of ~48 greater than that of the decoupled-poisoned moderator viewed by MaNDi at the FTS (at equal proton beam power). The sample-detector distance will be ~0.5 m. Figure 3.21 provides a schematic representation of the HiMaNDi instrument.

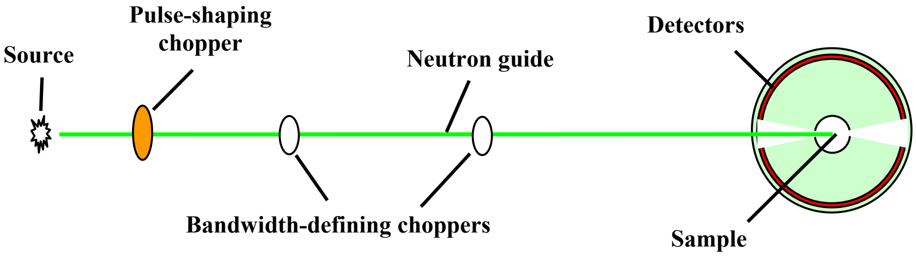

Fig. 3.21. Schematic representation of the HiMaNDi instrument.

The source pulse length at the STS is ~200-300 µs FWHM in the short-proton-pulse case and ~1000 µs in the long-proton-pulse case (1 ms proton pulse length). A high-speed "pulse-shaping" neutron chopper located at 8 m from the moderator will tailor the neutron pulse lengths as needed for the sample being studied. With a 130 m incident flight path, the neutron source pulse lengths for HiMaNDi in the short-proton-pulse case will provide adequate resolution for unit cell lengths of up to ~100 Å without using the pulse-shaping chopper, and the bandwidth will be 1.5 Å. The bandwidth available for MaNDi is 2.5 Å. The net data rate gain for HiMaNDi relative to MaNDi in the short-proton-pulse case is ~44 × 1.5/2.5 = 26. However, since HiMaNDi is designed to provide lower resolution than MaNDi, the HiMaNDi instrument placed on a coupled moderator at the FTS would have a gain relative to MaNDi of a factor of ~8 × 0.5/2.5 = 1.6 for measurements at this lower resolution. Therefore, the gain of HiMaNDi at the STS relative to HiMaNDi at the FTS would be a factor of ~16.5 in the short-proton-pulse case (at equal proton power for the FTS and the STS).

For the long-proton-pulse case, the pulse-shaping chopper will provide pulse lengths of 300 µs, and this chopping will reduce the time-averaged intensity from the STS moderator by a factor of ~3.3. This chopper will also limit the bandwidth available at the sample to ~0.5 Å for a single pulse. The net gain for HiMaNDi at the STS with one chopper pulse per source pulse relative to

HiMaNDi at the FTS would be a factor of ~5.5/3.3 = 1.7 for the long-proton-pulse case. However, with an incident flight path of 130 m, the STS 20 Hz pulse rate would allow a bandwidth of 1.5 Å. This is sufficient to accommodate three pulses in the long-proton-pulse mode through the chopper from each source pulse, tripling the data rate and providing gains of a factor of ~5 in data rate compared with HiMaNDi at the FTS (at the same source power). In reality, chopping efficiencies may make this gain factor a bit lower.

3.5.3.3 Very fast powder diffractometer for a small sampling volume

3.5.3.3.1 Science drivers

The study of atomic structure and transformations spans engineering materials, chemistry, condensed matter physics, geoscience, and biology. Current trends include increasing complexity (spatial inhomogeneity, symmetry lowering, large unit cells, multiple structure-property couplings, …), new length and time scales, increasing interest in deviations from long-range order, complex spin systems, more emphasis on organic and organic-containing materials, and more emphasis on kinetic measurements and parametric studies.

Many of the boundary-pushing experimental characteristics needed for such measurements cannot be provided by the current suite of U.S. materials diffractometers. Most of these needs can best be addressed by powder neutron diffractometers, which are extremely well suited to pulsed spallation sources. New instruments at the FTS would be most suitable for addressing some of these needs, but the high-intensity cold neutron beams and low repetition rate at the STS make it ideal for lower-resolution very fast powder diffractometers that are required to extend the ranges of kinetic measurements and expand the scope of parametric studies. Such instruments also permit the use of very small samples or small sampling volumes in larger samples. A Very-Fast Powder Diffractometer at the STS will provide these capabilities. This Very-Fast Powder Diffractometer will also be ideal for many experiments where d-spacings below 1 Å are not required, including moderate complexity crystallography, kinetics, phase transitions, spin structures, engineering materials, and mapping of orientation distribution functions. With the high intensity of long-wavelength neutrons, this diffractometer will also be excellent for the study of structures with very large d-spacings.

3.5.3.3.2 Instrument design and performance

The resolution required for this Very-Fast Powder Diffractometer is $\delta d/d = 5\times10^{-3}$ at $d \sim 2$ Å; and this sets $\delta\lambda/\lambda \sim 3.2\times10^{-3}$ at $\lambda \sim 3$ Å. Physical constraints at the STS limit the incident neutron beam path length for this instrument to a maximum of 130 m, and the sample-detector distance will be ~2 m. The pulse width for the coupled hydrogen moderators is ~200 μs at 3 Å [3.3] in the short-proton-pulse case, so with a 130 m flight path, the full pulse width can be used and still provide adequate resolution. For the long-proton-pulse case at the STS, a fast chopper at 8 m from the moderator will trim the pulse width to ~300 μs to give the desired resolution. Figure 3.22 provides a schematic representation of this Very-Fast Powder Diffractometer.

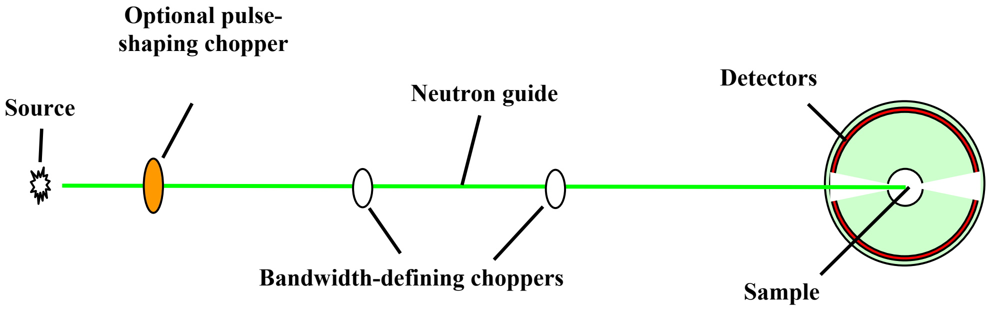

Fig. 3.22. Schematic representation of the Very-Fast Powder Diffractometer .

The coupled hydrogen moderators at the STS will produce a time-averaged neutron beam intensity factor of ~5.5 greater than that of the coupled hydrogen moderator at the FTS (at equal proton beam power), and the bandwidth at the short-proton-pulse version of the STS will be three times that at the FTS (1.5 vs 0.5 Å). This gives a total intensity gain of a factor of ~16.5 at the STS. In the long-proton-pulse version of this instrument at the STS, the pulse-shaping chopper will transmit a bandwidth of ~0.5 Å; but three pulses from this chopper can be used during each source pulse, so the net gain relative to the FTS in this case is a factor of ~5.

3.5.3.4 Magnetic studies powder diffractometer

3.5.3.4.1 Science drivers

The characteristics defined for the Very-Fast Powder Diffractometer are also well suited for the study of magnetic structures, including the behavior of such structures at high magnetic fields. However, different detector geometries and optimization of the sample area are required, so the STS will have a separate Magnetic Studies Powder Diffractometer. This instrument will be optimized for a wide variety of magnetic structural studies, including polarization analysis and including capabilities to accommodate very high magnetic fields at the sample.

3.5.3.4.2 Instrument design and performance

The main parameters for this instrument will be the same as for the Very-Fast Powder Diffractometer, except that the sample area will be optimized to accommodate polarized beam operation and one or more very-high-field magnets or other specialized configurations, and the detector locus will be optimized for the magnetic studies. The relatively long incident flight path provides another advantage for this instrument, since it needs to be situated far out to provide adequate lateral space to accommodate the magnet and to minimize stray magnetic field interference with other instruments. The instrument will look schematically much as is shown in Fig. 3.22, and the gains relative to a similar instrument at the FTS will be as described in Sect. 3.5.3.3.2.

3.5.4 Inelastic Scattering

3.5.4.1 Vertical surface resonance spin-echo spectrometer—reflectometer geometry

3.5.4.1.1 Science drivers

Inelastic/quasi-elastic neutron scattering is a unique tool for the investigation of dynamics because it gives a wave vector resolved access to the dynamics, which is essential to associate relaxation rates and excitation frequencies to specific motions and molecular components. Neutron spin-echo (NSE) is the spectroscopic method with the highest resolution in quasielastic and inelastic neutron scattering, with energy resolution values typically better than 10^{-5} of the incident neutron energy. Hence NSE spectroscopy is mainly used to study slow motions and relaxation phenomena in hard and soft condensed matter [3.14, 3.15]; these include much of the important dynamics in soft matter, biophysics, and biology. The large length scales involved usually require small Q-values.

Neutron reflectometry has recently made a quantum leap forward by going beyond the usual specular geometry. The investigation of off-specular scattering opens up a whole new field of phenomena. Furthermore, first experimental results show that a whole new field of surface excitations will be opened up by adding to a reflectometer the capability to discriminate between elastic and quasielastic scattering. Such an NSE reflectometer can also serve as a very low Q-range traditional NSE, since the access to the smallest Q-values in the order of 10^{-4} Å^{-1} will allow inelastic reflectometry and inelastic SANS. Such low Q values would not be accessible with conventional beam delivery approaches, since in that case NSE spectrometers run into high background issues around a scattering angle of ~5° and below. To adapt the Q-resolution to the particular experiment, a variable wavelength spread $\delta\lambda$ is necessary.

Since NSE is a Fourier technique, essentially all scattered neutron energies enter the spin analyzer and detector; therefore, only processes that contribute more than about ~5 % to the scattering intensity may be successfully analyzed. Inelastic scattering is usually much weaker than the elastic and quasi-elastic contributions and hence disappears in the counting statistics unless the instrument discriminates neutrons according to energy transfer. NSE was developed at reactor sources and was never combined with a dedicated TOF instrument. At spallation sources, however, NSE will obviously be combined with TOF. This combination will open up new possibilities, as a dedicated TOF NSE spectrometer would also allow for inelastic spin echo and studies of lifetimes of excitations with much greater resolution than is currently possible, relevant for example, for superconductors and quantum liquids.

Innovative design of the NSE instruments on the STS will extend the experimental capabilities of NSE beyond the existing limits and will allow for maximum flexibility as well as an overlap with other techniques. The needs in dynamic range and Q range, however, are so diverse and broad that they cannot be covered in an optimal way by a single instrument. To access very low scattering angles and large scattering angles in one instrument, a reflectometer-type instrument is needed. This instrument, referred to as the Vertical Surface Resonance Spin-Echo Spectrometer, has a horizontal scattering plane with a vertical sample geometry.

3.5.4.1.2 Instrument design and performance

This vertical surface "reflectometer" (for lack of a better word) will use an NRSE setup to minimize the weight of the echo components and the length of the spectrometer arms. Also, the NRSE configuration eliminates the need for the field integral correction elements used in conventional NSE, which have to be placed in the beam and are unwelcome. Moreover, the spectrometer arms can also be made shorter in the NRSE configuration.

The high-energy resolution is reached because in NSE or NRSE, the precession of neutron spins in a magnetic field measures directly the energy transfer at the sample and decouples the resolution from beam monochromatization and collimation. NSE and NRSE are Fourier methods that measure the intermediate scattering function $I(Q,t) = S(Q,t)/S(Q)$ in the limit $\hbar\omega << k_B T$. The relevant parameter is the Fourier time, $t \propto H\,\ell\,\lambda^3$, where H is the magnetic field ("effective" magnetic field in resonance spin-echo), ℓ the length over which the precession takes place, and λ the mean incident wavelength. The neutron bandwidth-limiting choppers on this TOF-NRSE spectrometer will essentially be run as for a reflectometer or diffractometer. The inelasticity of the scattering will be detected by the NRSE measurement, not by the difference of the neutron TOF from the elastic TOF. In this mode, the TOF discrimination is used only to minimize backgrounds.

However, to provide continuous coverage of a very large dynamical range of 6–7 orders of magnitude, this instrument will combine the spin-echo mode of operation ($\pi/2$ flippers ON) with a conventional chopper spectrometer inelastic scattering option at medium TOF resolution ($\pi/2$ flippers OFF), by including a high-speed chopper close to the sample. The NSE spectrometer at the Hahn-Meitner Institute (HMI) has very good experience with this mode [3.16]. This combination will extend the dynamical range by 1.5–2 orders of magnitude toward the low-resolution side. A TOF-NRSE spectrometer operating in the ranges (λ_{min}, λ_{max}), ($2\theta_{min}$, $2\theta_{max}$), ($H\ell_{min}$, $H\ell_{min}$) will cover a parameter range similar to that schematically shown in Fig. 3.23.

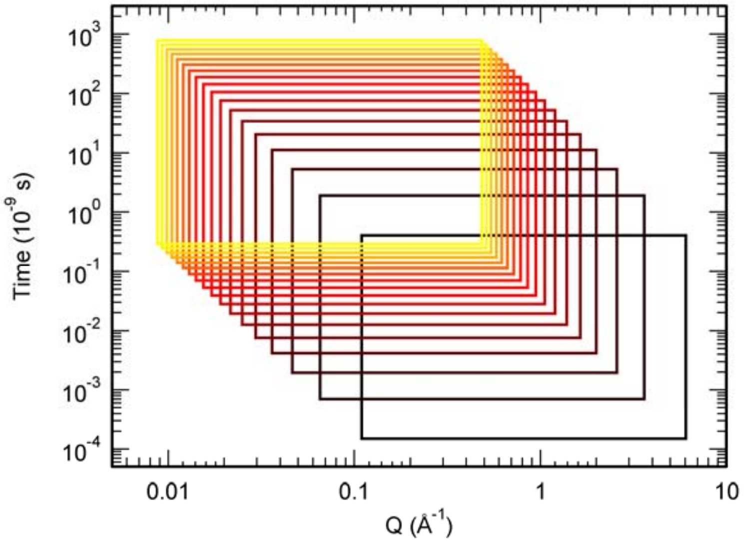

Figure 3.23. Range covered in a TOF-NRSE spectrometer. Here λ_{min}=2 Å (black), λ_{max}=25 Å (yellow), $2\theta_{min}$=2°, $2\theta_{max}$=150°, $H\ell_{min}$=100 Oe·cm, $H\ell_{max}$=270,000 Oe·cm. A time of 10^{-3} ns corresponds via Fourier transform to an energy transfer of 1 meV.

When comparing a location at different types of sources (reactor vs spallation source, long vs short pulse), one can omit the wavelength dependence of the intensity in first approximation because sources will be sufficiently similar in this respect. A figure of merit (FOM) will be proportional to the number of data points collected in unit time, divided by their squared errors. In first approximation, this would be given by the simple relation: FOM $\sim I \cdot P^2/B^2$ where I is the total intensity at the sample, B the background and P the polarization of the incident beam. The data points can be assumed to be equidistant on log scales in both Fourier time and Q vector. Hence the FOM will be proportional to the area of the covered range in Fig. 3.23, multiplied by the time-averaged intensity in each "pixel," which itself is proportional to the accepted wavelength spread $\delta\lambda$ in each "pixel." At a spallation source, this monochromaticity is given by the length of the incident beam line via $\delta\lambda$ (Å) = 4 δt (ms) / L (m), where δt is the initial length of the pulse; whereas at a reactor source, $\delta\lambda$ is in the 10–20 % range, depending on the velocity selector used. For a reasonable length of the spectrometer at a spallation source, $\delta\lambda$ can never be coarser than 5%; hence TOF resolution is virtually meaningless for NSE and NRSE. The FOM depends in part on the simultaneously covered wavelength range $\Delta\lambda$ [$\Delta\lambda$ (Å) = 4000/L (m)/ f (Hz)], with a large $\Delta\lambda$ giving a large area per instrument setting in Fig. 3.23, which is obviously preferred so long as the counting statistics do not vary too widely across the area.

The anticipated working range for this spectrometer is from $\lambda_{\min}$=2 Å to $\lambda_{\max}$=25 Å with peak use around 10 Å. This instrument will cover the range of scattering angles from $2\theta_{\min} = 0.1°$ to $2\theta_{\max} = 120°$, with $H\ell_{\min}$ = 100 Oe·cm, $H\ell_{\max}$ = 100,000 Oe·cm, and with a scattered flight path length of ~1.5–2 m. It will have a source-to-sample distance of L ~40 m. None of these numbers limiting the ranges are pushing current instrumental limits. Figure 3.24 shows this instrument schematically.

For f=20 Hz and with an incident proton beam power (short-proton-pulse or long-proton-pulse) of 1 MW, the performance for this instrument estimated by scaling from the reflectometer and spin echo beam lines at the FTS is

wavelength resolution $\delta\lambda \sim 0.1$ Å
wavelength bandwidth $\Delta\lambda \sim 5$ Å
neutron flux on sample in the band 2–7 Å: ~ 4×10^9 n·cm^{-2}·s^{-1}
neutron flux on sample in the band 7–12 Å: ~ 7×10^8 n·cm^{-2}·s^{-1}

These flux values are about a factor of 16.5 times those that would be available for an equivalent instrument at the FTS (for 1 MW on the FTS). This is roughly due to a factor of 5.5 for the time-averaged flux and a factor of 3 for the simultaneously covered bandwidth (20 Hz vs 60 Hz). Note that the guide must terminate outside the first precession region, and this limits the divergence incident on the sample to ~± 2°.

Figure 3.25 shows the Q-t range spanned by this instrument.

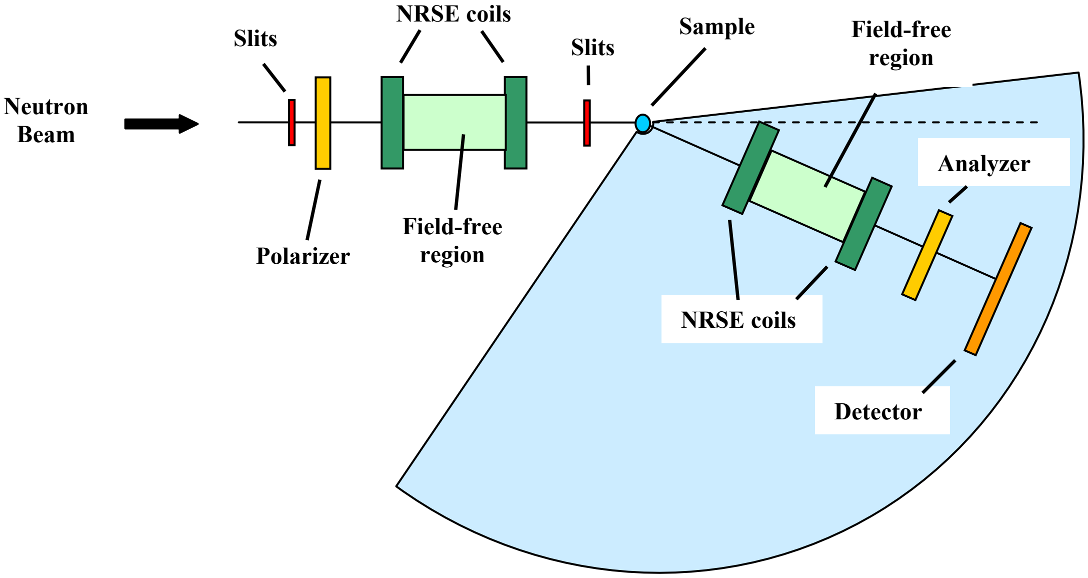

Fig. 3.24. Schematic plan view of the Vertical Surface Resonance Spin-Echo Spectrometer. The scattered beam measurement arm swings around through the shaded arc shown. The incident beam has a neutron guide, bandwidth choppers, and optional high-speed TOF chopper, which are not shown in this view.

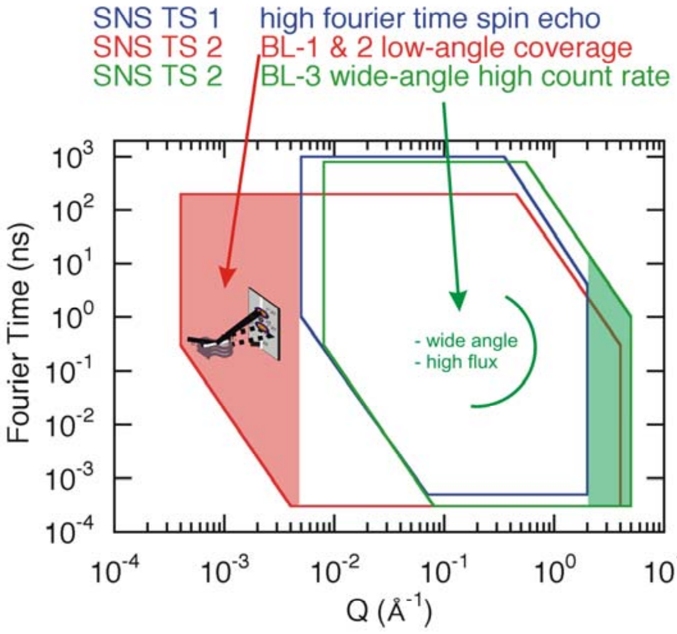

Figure 3.25. Ranges in the spatial and temporal variables covered by the three proposed NRSE instruments. Here SNS TS 1 refers to the high-resolution NSE instrument at the FTS, SNS TS 2 BL-1, BL-2, and BL-3 refer to the vertical-surface, horizontal-surface, and wide-angle STS NRSE instruments, respectively. Note the gain in low Q-values as compared with existing NSE instruments.

3.5.4.2 Horizontal surface resonance spin-echo spectrometer—reflectometer geometry

3.5.4.2.1 Science drivers

The Horizontal Surface Resonance Spin-Echo Spectrometer is designed to meet the requirements for the investigations of liquids and free-standing surfaces with a horizontal sample and a vertical scattering plane. It will be complementary to the Vertical Surface Resonance Spin-Echo Spectrometer (Sect. 3.5.4.1), and most of the science drivers from Sect. 3.5.4.1.1 also apply to this instrument. The access to smallest Q-values in the order of 10^{-4} $Å^{-1}$ will allow inelastic reflectometry and inelastic SANS on this instrument as well. Because of the large structures involved in biophysics and biology, this range of length and time scales is extremely interesting. Previous information about dynamics on these long length scales mainly stems from analysis of diffuse scattering with the inherent drawback that underlying Q-information is lost. This small-angle NRSE instrument with a horizontal sample stage will innovate the investigation of liquids and allow dynamical investigation of liquid surfaces and interfaces. The impact here is to study propagating modes in biophysics and biology and their importance for biological key functions. To adapt the Q-resolution to the particular experiment, a variable wavelength spread $\delta\lambda$ is necessary.

3.5.4.2.2 Instrument design and performance

The design of much of this instrument will be virtually the same as for the Vertical Surface Resonance Spin-Echo Spectrometer, with the following exceptions:

- The horizontal-surface-reflectometer sample geometry is necessary for the study of free-standing liquid surfaces.
- This sample geometry requires a vertical scattering plane, which restricts the range of scattering angles that can be covered.
- This geometry also requires a downward-sloping incident beam.

The anticipated working range for this spectrometer is from λ_{min}=2 Å to λ_{max} = 25 Å with peak use around 10 Å. This instrument will cover the range of scattering angles from $2\theta_{min} = 0.1°$ to $2\theta_{max} = 90°$, with $H\ell_{min}$ = 100 Oe·cm, $H\ell_{max}$ = 100,000 Oe·cm and with a scattered flight path length of ~1.5–2 m. It will have a source-to-sample distance of L ~40 m. None of these numbers limiting the ranges is pushing current instrumental limits. Figure 3.5.26 shows this instrument schematically.

For f=20 Hz and with incident proton beam power (short-proton-pulse or long-proton-pulse) of 1 MW, the performance for this instrument estimated by scaling from the reflectometer and spin-echo beam lines at the FTS is

wavelength resolution $\delta\lambda$ ~0.1 Å
wavelength bandwidth $\Delta\lambda$ ~5 Å
neutron flux on sample in the band 2–7 Å: ~ 4×10^{9} $n\cdot cm^{-2}\cdot s^{-1}$
neutron flux on sample in the band 7–12 Å: ~ 7×10^{8} $n\cdot cm^{-2}\cdot s^{-1}$

These flux values are about a factor of 16.5 times those that would be available for an equivalent instrument at the FTS (for 1 MW on the FTS). This is based on a factor of 5.5 for the time-averaged flux and a factor of 3 for the simultaneously covered bandwidth (20 Hz vs 60 Hz).

Note that the guide must terminate outside the first precession region, and this limits the divergence incident on the sample to ~± 2°.

Figure 3.26 shows the Q-t range spanned by this instrument.

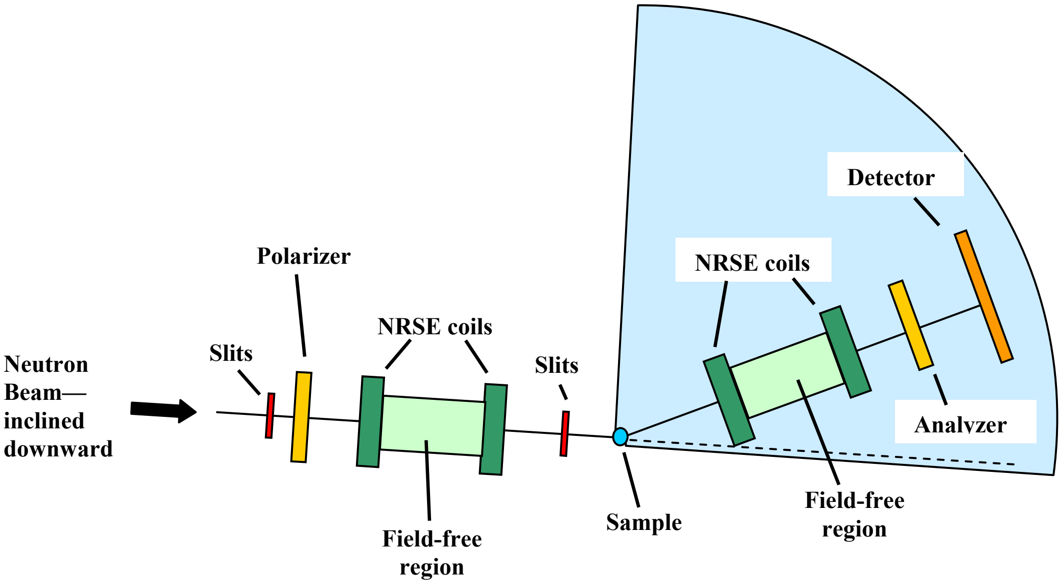

Fig. 3.26. Schematic elevation view of the Horizontal Surface Resonance Spin-Echo Spectrometer. The scattered beam measurement arm swings around through the shaded arc shown. The incident beam has a neutron guide, bandwidth choppers, and optional high-speed TOF chopper, which are not shown in this view.

3.5.4.3 Wide-angle NRSE spectrometer

3.5.4.3.1 Science drivers

In addition to the two “reflectometer-geometry” NRSE instruments (Sects 3.5.4.1 and 3.5.4.2), there is also a need for a wide-angle NRSE instrument to provide dynamical measurements simultaneously over a broad band of length scales. Most of the science drivers from Sect. 3.5.4.1.1 also apply to this instrument; in addition, it will provide the capabilities necessary to study the kinetic evolution of the slow dynamical processes in a wide range of materials. As for the other two NRSE instruments, this instrument will also be provided with TOF capabilities to extend the dynamical range.

3.5.4.3.2 Instrument design and performance

The anticipated working range for this spectrometer is from λ_{min}=2 Å to λ_{max} = 25 Å with peak use around 10 Å. This instrument will simultaneously cover the range of scattering angles from $2\theta_{min} = 5°$ to $2\theta_{max} = 150°$, with $H\ell_{min}$ = 100 Oe·cm, $H\ell_{max}$ = 270,000 Oe·cm and with a scattered flight path length of ~2.5–3 m. It will have a source-to-sample distance of L ~40 m and will have a much larger guide cross-section than is the case for the two reflector-geometry NRSE instruments. None of these numbers limiting the ranges is pushing current instrumental limits. Figure 3.27 shows this instrument schematically.

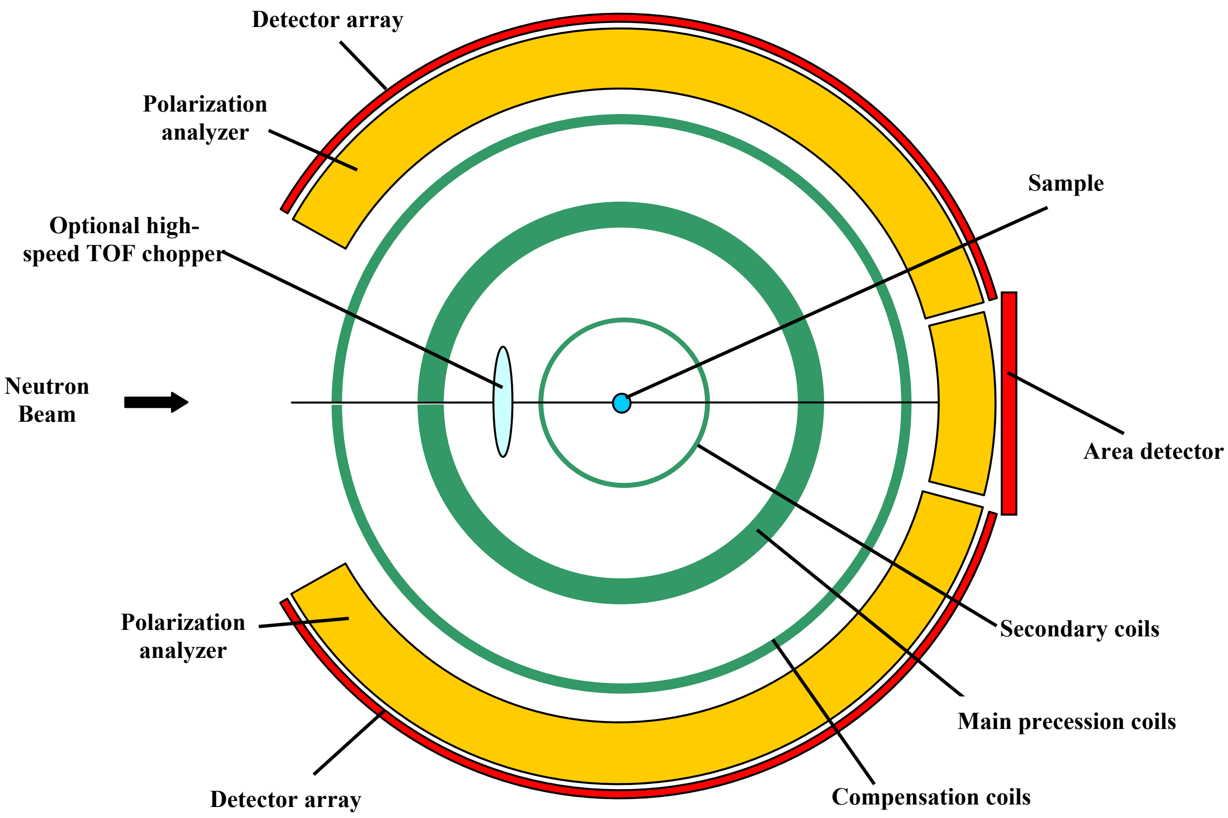

Fig. 3.27. Schematic plan view of the Wide-Angle NRSE Spectrometer. The incident beam has a neutron guide, bandwidth choppers, and optional high-speed TOF chopper. Of these, only the high-speed TOF chopper is shown in this view.

For *f* = 20 Hz and with incident proton beam power (short-proton-pulse or long-proton-pulse) of 1 MW, the performance for this instrument estimated by scaling from the reflectometer and spin-echo beam lines at the FTS is

wavelength resolution $\delta\lambda$ ~0.1 Å
wavelength bandwidth $\Delta\lambda$ ~5 Å
neutron flux at sample in the band 2–7 Å: ~ 8×10^{8} $\mathrm{n\cdot cm^{-2}\cdot s^{-1}}$
neutron flux at sample in the band 7–12 Å: ~ 7×10^{7} $\mathrm{n\cdot cm^{-2}\cdot s^{-1}}$

These flux values are about a factor of 16.5 times those that would be available for an equivalent instrument at the FTS (for 1 MW on the FTS). This is roughly due to a factor of 5.5 for the time-averaged flux and a factor of 3 for the simultaneously covered bandwidth (20 Hz vs 60 Hz). Note that the guide must terminate outside the first precession region, and this limits the divergence incident on the sample to ~± 1°.

Figure 3.27 shows the Q-t range spanned by this instrument.

3.5.4.4 High-resolution backscattering spectrometer

3.5.4.4.1 Science drivers

Backscattering spectrometers (“indirect geometry”) can provide the highest energy resolution of any of the non-spin-echo spectrometers. However, they are not as flexible as the direct geometry spectrometers such as the chopper spectrometers and crystal monochromator spectrometers, some of which can provide better Q-resolution than can the backscattering spectrometers. Nevertheless, because of the excellent energy resolution, a backscattering spectrometer will be an important component of a comprehensive suite of inelastic scattering spectrometers.

Scientific applications for which the high resolution of the backscattering spectrometer will be particularly important include the study of interfacial dynamics, dynamics of biological samples, observations of the dynamics of adsorption and of molecules in confined geometries, tunneling spectra, dynamics of glassy systems, and diffusive processes in ionic and proton conductors. Other areas in which this spectrometer will play a significant role include quantum magnetism, molecular magnetism, frustrated magnets, relaxor ferro-electrics, and a variety of phenomena associated with energy storage.

3.5.4.4.2 Instrument design and performance

The design of the High-Resolution Backscattering Spectrometer is similar to that proposed in the ESS design [3.17]. This design has a 130 m moderator-to-sample distance and a 4 m sample-to-detector distance. Stressed Si(111) analyzer crystals in exact backscattering would provide 800 neV resolution at zero energy transfer. To achieve this resolution level, a Fermi pulse-shaping chopper is used to control the moderator contribution to the resolution function. This chopper must restrict the pulse width to ~30 μs in order to achieve the highest resolution. If such a chopper is placed at 8 m from the moderator on a short-proton-pulse source, it will transmit a bandwidth of ~0.15 Å, which translates to a dynamic range of ~± 50 μeV about the elastic line; whereas the same chopper on a long-proton-pulse (1 ms) source will transmit a bandwidth of ~0.5 Å, giving a dynamic range of ~± 160 μeV. In either case, this instrument would have a maximum Q of 1.9 $Å^{-1}$. The pulse-shaping chopper can also be used to relax the resolution to 4 μeV if more flux is required. At 1 MW on the STS, the useful flux on sample in the high-resolution case will be $\sim 5\times10^6$ $n/cm^2/s$ for either source case, provided the entire dynamic range is useful. This is about a factor of 5.5 more than would be possible with a similar instrument on the coupled cold moderator at the FTS (for 1 MW on each source) because of the factor of 5.5 difference in cold-neutron intensity between the FTS and the STS coupled moderators. Since the accessible bandwidth is limited by the pulse-shaping chopper, the lower source frequency on the STS does not provide any gains when only one chopper pulse per source pulse is used. However, further optimization of this instrument using wavelength frame multiplication may permit the use of more than one chopper pulse per source pulse, changing these ratios in cases where the broader bandwidth would be useful.

Figure 3.28 provides a schematic representation of this instrument.

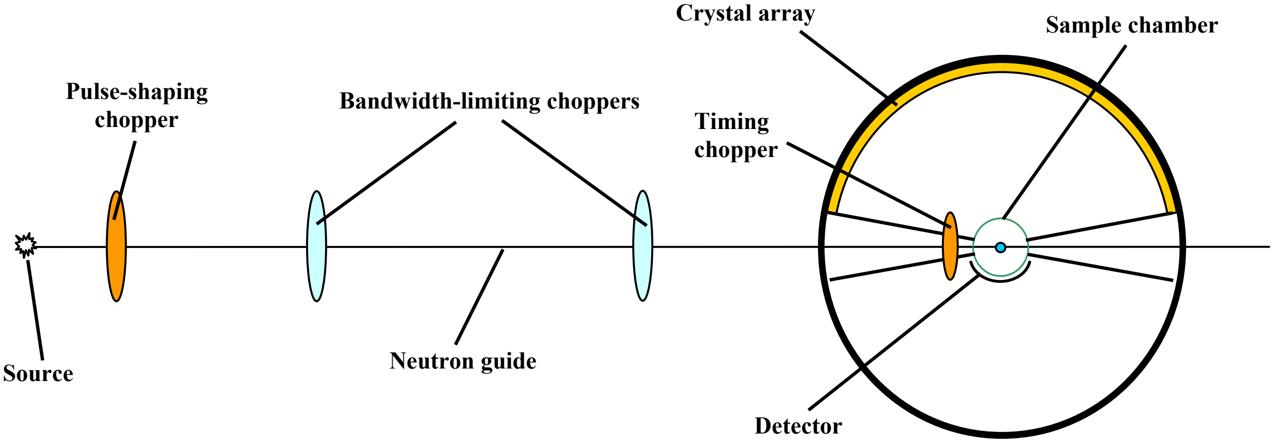

Fig. 3.28. Schematic plan view of the High-Resolution Backscattering Spectrometer. The timing chopper discriminates against neutrons scattered directly from the sample to the detectors.

3.5.4.5 High-resolution cold neutron chopper spectrometer

3.5.4.5.1 Science drivers

The High-Resolution Cold Neutron Chopper Spectrometer will be a highly versatile and flexible instrument with applicability to a wide variety of scientific problems. These include the study of interfacial dynamics, dynamics of biological samples, observations of the dynamics of adsorption and of molecules in confined geometries, tunneling spectra, dynamics of glassy systems, and diffusive processes in ionic and proton conductors. Other areas where such spectrometers will play a significant role include quantum magnetism, molecular magnetism, frustrated magnets, relaxor ferro-electrics, and a variety of phenomena associated with energy storage. Furthermore, it can address other problems ranging from membrane collective dynamics to ferro-elastic modes in shape-memory alloys. Many of these are the same areas indicted for the backscattering spectrometers, since there is significant overlap in the energy resolution ranges. However, the Cold Neutron Chopper Spectrometer can also use much higher incident energies than can the backscattering spectrometer and so can access a much broader Q range (range of length scales). It cannot reach to the lowest energy resolutions accessed by the backscattering spectrometer, but it can provide better Q resolution than can the backscattering spectrometer.

3.5.4.5.2 Instrument design and performance

The High-Resolution Cold Neutron Chopper Spectrometer uses a pulse-shaping chopper to select a narrow (in time) pulse of neutrons from the peak of the broader neutron pulse supplied by the source. This leads to a preference for such a chopper spectrometer to be on a short-proton-pulse source if equal power is provided by the long-proton-pulse counterpart.

A Cold Neutron Chopper Spectrometer (CNCS) already being constructed at the FTS has an elastic resolution of 1% of the incident energy. The main gains at a short-proton-pulse STS arise from a factor of 6 increase in peak flux compared with the FTS (at 1 MW on each source) and the use of repetition rate multiplication (RRM) [3.18]. RRM relies on the flight paths remaining fairly long to avoid frame-overlap issues. The moderator to high-speed chopper distance of ~30 m for this instrument allows RRM gains of approximately 3 to 5. Total gains in data rate for the short-proton-pulse STS are thus between 16.5 and 27.5 times the CNCS at the FTS (at 1 MW). These must be multiplied by a factor of ~0.3 for a long-proton-pulse (1 ms) STS at equal power. Figure 3.29 provides a schematic representation of the main components of this spectrometer.

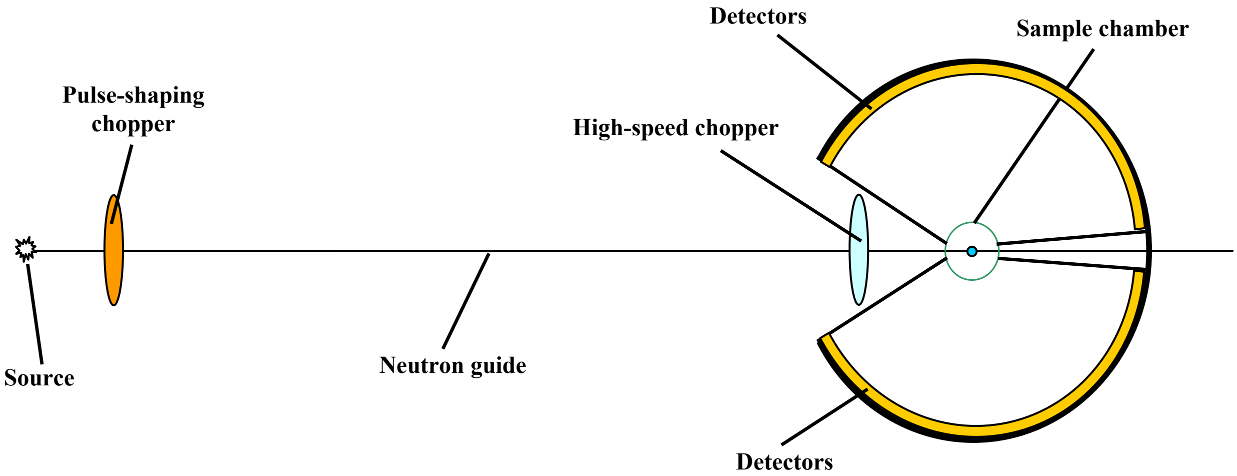

Fig. 3.29. Schematic plan view of the High-Resolution Cold Neutron Chopper Spectrometer .

A simple timing diagram showing RRM for the case of three incident energies, E_i, of 2, 1.36, and 0.94 meV, (solid green lines) is given in Fig. 3.30. With the moderator at the origin, the sample located 36 m downstream (dotted black line), and a 4 m final flight path to the detectors (dashed black line), a final energy of 0.15 times E_i (red lines), and 2 times E_i (blue lines), this figure shows no frame overlap.

An increased duty cycle may be described by a case of E_i = 10.0, 6.6, 4.4, 2.9 and 1.9 meV where approximately five independent experiments (in terms of resolution and dynamics range) could be performed simultaneously (Fig. 3.31). New concepts in data reduction must also be broached in cases such as these where the interesting scientific features are simultaneously measured at multiple resolutions. This instrument will be designed to accommodate polarized beam experiments and to allow sufficient flexibility for ancillary equipment around the sample position.

3.5.4.6 High-intensity cold neutron chopper spectrometer

3.5.4.6.1 Science drivers

The High-Intensity CNCS will be able to address many of the same types of systems as studied by the High-Resolution CNCS, but the emphasis will be on lower-resolution measurements with much smaller samples (e.g., as demanded by extreme sample environments) or on high data rates that permit kinetic measurements with short-time-constant phenomena. The high data rates will also be important for pump-probe experiments to follow relaxations with much shorter time constants than were previously accessible, and for extensive parametric studies.

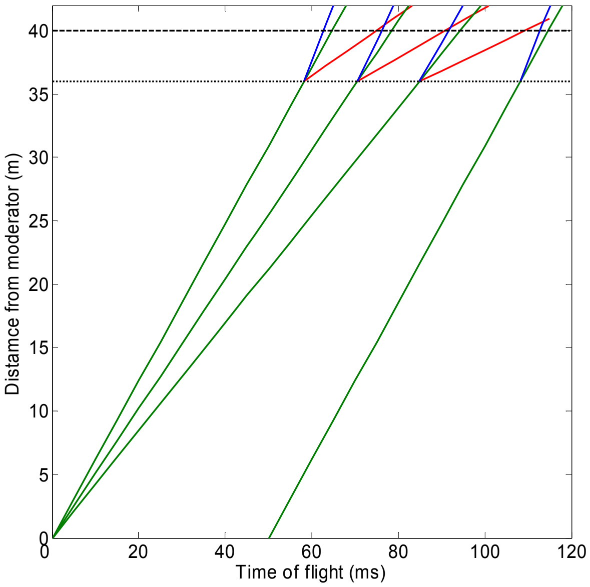

Fig. 3.30. Timing diagram showing a possible repetition-rate-multiplication scheme. Here Ei = 2, 1.36, and 0.94 meV for a cold neutron chopper spectrometer at a 20 Hz source.

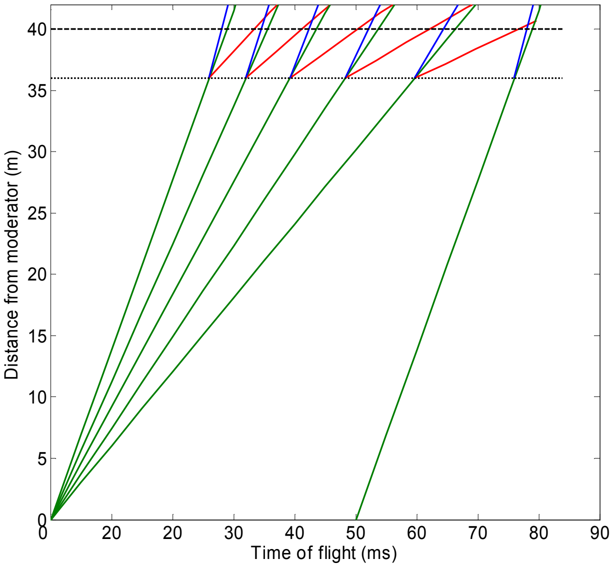

Fig. 3.31. Timing diagram showing another possible RRM scheme. Here Ei = 10, 6.6, 4.4, 2.9, and 1.9 meV for a cold neutron chopper spectrometer at a 20 Hz source.

3.5.4.6.2 Instrument design and performance

This instrument will have a similar design and similar dimensions to those for the High-Resolution CNCS and will look schematically as shown in Fig. 3.29. However, the resolution requirements will be relaxed to ~5% of the incident energy, in which case no pulse shaping (short-proton-pulse version) or only minimal pulse shaping (long-proton-pulse version) will be required. This factor of 5 poorer resolution will result in flux gains of a factor of ~25 relative to that of the High-Resolution CNCS. Together with RRM, the flux on the sample in this instrument will be a factor of 16.5 to 27.5 times that of the CNCS at the FTS (at 1 MW) in the short-proton-pulse case. The pulse-shaping chopper selects a 500 μs long pulse in the long-proton-pulse case, so these data rate gain factors must be reduced by a factor of ~2 for a long-proton-pulse (1 ms) STS at equal power. To further enhance the data rates for very small samples, this instrument will incorporate a focusing optic that can be inserted into the incident beam just before the sample as needed, and this will be able to provide up to an additional order of magnitude in flux. The combined 2 orders of magnitude in flux relative to the CNCS will revolutionize areas of science where small sample volumes are predominant.

If there is sufficient demand, a second such instrument might be optimized for and dedicated to experiments with one or two different types of extreme environment equipment (e.g., ultra-high pressures or ultra-high-field magnets). Extreme sample environments are notorious for constricting sample volumes and/or for restricting the available solid angle to detect the scattered neutrons. The use of focusing optics to provide a micron-sized, focused beam could effectively allow for inelastic scattering to be measured from samples under giga-Pascal pressures, under relatively fast changing stimulus, or even under high magnetic fields.

The key to such a spectrometer would be building the sample environment into the spectrometer design. Significant economy could be achieved over a traditional spectrometer by tailoring the detector layout to be suitable for the sample geometry.

3.5.5 Imaging

3.5.5.1 Neutron imaging beamline

3.5.5.1.1 Science drivers

The neutron imaging beamline will enable new science, including rapid 3-dimensional and time-resolved imaging and better sensitivity to composition and thickness resulting from the use of longer wavelength neutrons. Optics to attain much higher spatial resolution are possible with the longer-wavelength neutrons, and sharper images may be possible with the use of TOF to separate the contributions from different wavelengths. The use of TOF also facilitates Bragg edge imaging techniques to provide material-selective contrast. This beamline will also provide the capability of doing large-field tomography with the ability to "zoom in" and do more discrete measurements at higher resolution. The high flux of cold neutrons available at the imaging beamline will provide new capabilities for real-time process monitoring and for time-resolved measurements of processes in areas as diverse as the crystallization or decomposition of minerals at high temperatures and pressures; rheology in fluids and melts, including measurements under high pressure and temperature conditions; the transport of lubricants through operating machinery; or the transport of water in a variety of systems ranging from plant root systems to fuel cells.

The techniques made possible with this instrument will find applicability across a broad spectrum of scientific areas, including most of the general areas listed in Chapter 2.

3.5.5.1.2 Instrument design and performance

This instrument is a configurable multipurpose beamline that combines direct imaging, phase contrast methods, radiography, residual stress, and microscopy into a single "instrument." The optical requirements for these measurements are sufficiently similar without significant compromise of any particular capability. The common geometry that defines this instrument is the use of pinhole optics and the provision of a long aperture-to-sample flight path (~30 m) to allow imaging of large samples when desired. This highly-flexible evacuable flight path is adjustable to provide shorter pinhole-to-sample distances when desired, or to include optical benches and sample and detector mounts positioned at various distances from the aperture. A rotating collimator provides remotely selectable pinhole apertures with different diameters, and there is a provision to install converging optics or other specialized optics upstream from these apertures. Figure 3.32 provides a schematic representation of this imaging beamline at the STS.

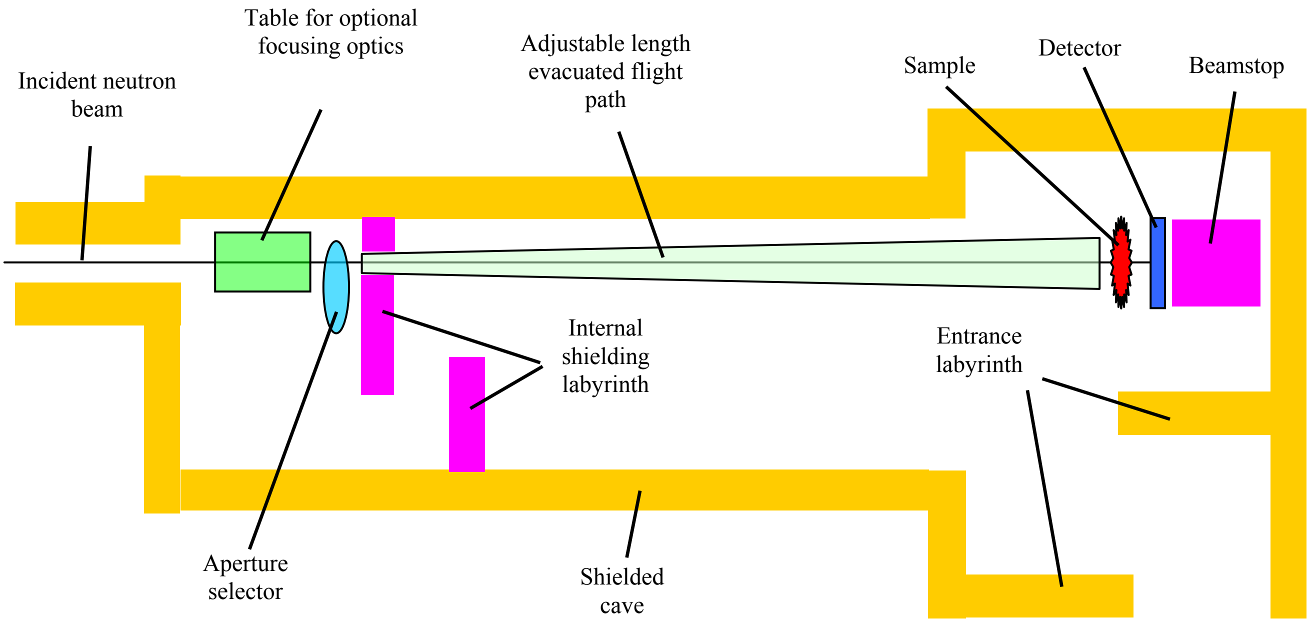

Fig. 3.32. Schematic plan view of the imaging beamline. The incident beam has a curved neutron guide and bandwidth choppers that are not shown in this view. The entrance labyrinth is sufficiently large to bring large samples or other equipment into the cave when desired.

The distance from the source to the pinhole aperture will be ~20 m to provide sufficient distance to curve the beam out of the fast-neutron line-of-sight. Bandwidth choppers located within this 20 m section will eliminate frame overlap and will allow operation in different frames when desired. At 20 m from the source, there will be adequate space between neighboring beams to permit a sufficiently large shielded cave to provide room for the desired flexibility.

This instrument will have approximately a factor of 5.5 more source intensity at the STS than if it were built at the FTS, and it will have another gain factor of ~3 from the lower repetition rate at the STS, resulting in a total data rate gain factor of ~16.5 relative to the FTS. This will be the same for either the short-proton-pulse or long-proton-pulse option. With the high degree of flexibility and sufficient space in the cave, it will be possible also to incorporate simultaneous measurements with other techniques, such as prompt gamma and X-ray imaging (image fusion), light and electron microscopy and spectroscopy, X-ray fluorescence, X-ray diffraction, polarimetry, rheometry, or ultrasound, etc., to further enhance the science that can be conducted.

3.5.6 Fundamental Neutron Physics

3.5.6.1 Ultra-cold neutron beamline

3.5.6.1.1 Science drivers

An intense pulsed source such as the STS offers a particular opportunity for fundamental neutron physics. Measurements in this field are almost always significantly limited by statistical and systematic effects. A pulsed source offers a particular advantage in the identification of systematic errors. For the ultra-cold neutron (UCN) beamline, the advantages of the STS in reducing systematic errors lie in two main areas:

1. Using developments in neutron guide technology, particularly curved "benders" to transport the beam far away from other equipment and experiments without significant loss of flux, thereby reducing gamma-ray and neutron backgrounds. The proposed external UCN facility will be far from other instruments.
2. The design of an independent external experimental facility allows the opportunity to address seismic/vibration noise that is particularly important for some experiments with UCNs.

Experiments with this beamline will include the search for a neutron electric dipole moment and the measurement of the neutron lifetime.

3.5.6.1.2 Instrument design and performance

The STS does not have the capability to directly produce beams of UCNs, but there are several proposed experiments that accept neutrons with a wavelength of ~8.9 Å and convert them to UCN in the experimental apparatus. Such experiments benefit from a large-cross-section large-divergence beam. The UCN beamline at the STS will use a fully optimized ballistic guide. At this beamline, one can expect an increase in beam intensity from improved optics alone (P. Huffman, North Carolina State University. Personal communication with G. L. Greene, ORNL, 2006) of nearly an order of magnitude relative to the nEDM experiment at the FTS. The intensity gain over the STS optimized cold source will provide an additional gain factor of ~5.5 relative to the FTS cold coupled moderator. The total 60-fold increase relative to the nEDM experiment at the FTS in flux will qualitatively change the science that is attainable. However, because it uses only a narrow wavelength band the UCN beamline will not benefit from the wider bandwidth at the STS, except perhaps indirectly from the lower background due to longer periods between pulses. Therefore, the gain factor of the UCN beamline relative to a comparably optimized UCN beamline at the FTS will be only the factor of ~5.5 from the source brightness.

3.5.7 Summary of the Reference Instrument Suite

Table 3.4 summarizes the major parameters and the estimated performance for the reference or straw man instruments suite described in Sects. 3.5.1 through 3.5.6. It is evident from Table 3.4 that all of the reference instruments so selected show very large gains at the STS compared with the FTS, with the gains for most being well over an order of magnitude. Table 3.4 also shows the beamline chosen for each instrument for the reference STS facility configuration.

Table 3.4. Reference instrument suite

	Instrument	Beamline	Source–sample distance (m)	Sample–detector distance (m)	Gain relative to FTS short pulse (long pulse) *
SANS					
3.5.1.1	High-Throughput SANS	13	20	≤ 12	16.5 (16.5)
3.5.1.2	Biology SANS	14	20	≤ 12	16.5 (16.5)
3.5.1.3	High-Resolution SANS	12	26	≤ 18	16.5 (16.5)
3.5.1.4	Spin-Echo SANS (SESANS)	18	24	≤ 10	16.5 (16.5)
Reflectometry					
3.5.2.1	High-Intensity Horizontal-Surface Reflectometer	15	30	≤ 2	11 (11)
3.5.2.2	High-Intensity Vertical-Surface Reflectometer	9	30	≤ 3	11 (11)
3.5.2.3	Grazing-Incidence Diffraction (GID) and Grazing-Incidence SANS (GISANS) Instrument	16	30	≤ 5	11 (11)
3.5.2.4	Spin-Echo Resolved Grazing Incidence Spectrometer (SERGIS)	19	24	≤ 3	11 (11)
Diffraction					
3.5.3.1	High-Resolution Low-Q Neutron Diffractometer	4	75	3	16.5 (5)
3.5.3.2	High-Throughput Single-Crystal Macromolecular Diffractometer (HiMaNDi)	8	130	0.5	16.5 (5)
3.5.3.3	Very-Fast Powder Diffractometer	7	130	2	16.5 (5)
3.5.3.4	Magnetic Studies Powder Diffractometer	6	130	3	16.5 (5)
Inelastic Scattering					
3.5.4.1	Vertical-Surface Resonance Spin-Echo Spectrometer	2	40	2	16.5 (16.5)
3.5.4.2	Horizontal-Surface Resonance Spin-Echo Spectrometer	17	40	2	16.5 (16.5)
3.5.4.3	Wide-Angle Neutron Spin Echo Spectrometer	3	40	3	16.5 (16.5)
3.5.4.4	High-Resolution Backscattering Spectrometer	5	130	4	5.5 (5.5)
3.5.4.5	High-Resolution Cold Neutron Chopper Spectrometer	11	30	4	16.5 (5)
3.5.4.6	High-Intensity Cold Neutron Chopper Spectrometer	10	30	4	16.5 (8)
Imaging					
3.5.5.1	Imaging Beamline	1	20	30	16.5 (16.5)
Fundamental Neutron Physics					
3.5.6.1	Ultra-Cold Neutron Beamline	20	40	–	5.5 (5.5)

* Assumes long-proton-pulse time-averaged power = short-proton-pulse time-averaged power = FTS time-averaged power.

Table 3.5 shows the set of instruments that are shown in Table 2.1 as being necessary to carry out the full scientific agendas elucidated in Sects. 2.1.1 through 2.1.8, but it now shows both the areas covered by presently-planned FTS instrumentation and those covered by the STS reference instrument suite. From this comparison, it can be seen that the STS instrumentation will be complementary to that at the FTS, and that between the two facilities, most of the suggested instrumentation is addressed. Not apparent in the table, but clear from the analyses in Sects. 3.5.1 through 3.5.6, is that in some of the areas where there is overlap, the STS instrument performs much better than its FTS counterpart. This opens the option of replacing some of the FTS instruments with different types of instruments much better suited to the FTS characteristics, leading to even greater scientific productivity.

In addition to the capabilities shown in Table 3.5, several of the STS reference instruments provide capabilities that were not envisioned at the time when the scientific studies on which this table is based were carried out. These include the ability to reach lower Q values in SANS measurements by using the SESANS technique (3.5.1.3); the ability to study in-plane structures in thin films or membranes and at interfaces using the GISANS, GID, or SERGIS techniques (3.5.2.3, 3.5.2.4); and the ability to probe low-energy dynamics at lower Q-values by combining the NRSE technique with a reflectometer geometry (3.5.4.1, 3.5.4.2).

Table 3.5. Neutron beam instrumentation required for next-generation science—FTS and STS

Type	Instrument	Section requesting instrument							
		2.1.1	2.1.2	2.1.3	2.1.4	2.1.5	2.1.6	2.1.7	2.1.8
SANS									
	High-resolution focusing small-angle-scattering instrument		X	X	X				
	High-intensity SANS			X	X	X			
	High-resolution SANS optimized for biology						X		
	High-intensity SANS optimized for biology						X		
Reflectometry									
	Polarized neutron reflectometer with high Q resolution and high intensity		X	X					
	High-intensity reflectometer			X	X				
Diffraction									
	Powder diffractometer with 0.1% d resolution	X	X	X					
	High-intensity powder diffractometer	X	X	X					
	Engineering diffractometer for stress-strain analysis		X						
	Diffuse scattering diffractometer with full polarization analysis		X		X				
	Good resolution powder diffractometer covering length scales up to nm	X	X	X	X				
	Small-unit-cell single crystal diffractometer	X		X					
	Magnetic powder diffractometer	X		X					
	Single-pulse diffractometer		X	X					
	Liquids diffractometer				X	X			
	Intense, focused-beam protein crystallography diffractometer for small crystals						X		
	Intense, larger-beam long-wavelength crystallography diffractometer for higher-molecular weight crystals at high resolution						X		
	Extreme environment diffractometer(s) for high P and T							X	

Table 3.5. (continued)

	Instrument to perform simultaneous phase, structure, texture, and stress analyses under high P and T conditions							**X**	
Inelastic Scattering									
	🟩 High-resolution backscattering spectrometer	**X**	**X**	**X**	**X**	**X**	**X**		
	Lower-resolution backscattering spectrometer with Q up to 5 $Å^{-1}$	**X**					**X**		
	🟩 Variable-resolution cold neutron chopper spectrometer	**X**	**X**	**X**	**X**	**X**	**X**		
	🟦 Thermal chopper spectrometer	**X**		**X**		**X**	**X**		
	🟦 High-energy chopper spectrometer	**X**		**X**		**X**			
	🟩 High-resolution neutron spin-echo spectrometer			**X**	**X**	**X**	**X**		
	🟨 Wide-angle spin-echo spectrometer				**X**	**X**	**X**		
	🟨 One or more inelastic spectrometers dedicated to (or at least useable for) ultra-high P and T measurements							**X**	
Imaging									
	🟨 Tomography and radiography instrument using time-of-flight to identify different components and phases		**X**					**X**	
Fundamental Neutron Physics									
	🟩 Beamline dedicated to Ultra Cold Neutron production								**X**
	🟦 Beamline for neutron decay studies								**X**
	🟦 Cold beamline for neutron optics studies including interferometry								**X**

🟦	An instrument at the FTS is available or is being built to satisfy most of these requirements.
🟩	An FTS instrument is available or planned, but an STS reference instrument provides capabilities beyond those of the FTS instrument.
🟨	An STS reference instrument addresses most of these requirements.

X Instrument requested in Sects. 2.1.1 through 2.1.8.

3.6 CONCEPTUAL LAYOUT OF THE STS FACILITY WITH REFERENCE INSTRUMENT SUITE

Figure 3.33 shows the layout on the SNS site of the STS Target Building, instruments, and associated new infrastructure. The location of the target building is an evolution from the original plan for a second target building identical to the first one. To accommodate longer beam lines appropriate for this type of facility, the target building was shifted to near the ellipse road to allow long beam lines on the opposite side. This arrangement also minimizes the site work required for the large level areas of undisturbed soil needed for minimum settlement of new structures.

The existing Central Utilities Building (CUB) and associated cooling towers are projected to be at their maximum capacity for tower water, chilled water, hot water, and compressed air after the PUP is complete. A new CUB and associated cooling towers will be required to provide these utilities to the new facilities proposed. There is no excess capacity in the existing Central Exhaust Facility (CEF) so a new CEF will be required for primary confinement exhaust, secondary confinement exhaust, hot off–gas, and tunnel exhaust.

Significant site work will be required to relocate the approximately 150,000 yd^3 of excess soil located on the site of the new target building. Extensive underground utilities will be installed to the new facilities.

New offices are planned as an extension to the existing Central Lab and Office Building (CLO) to optimize existing usage of current infrastructure. New laboratories are planned as a standalone building because of lack of space adjacent to the existing CLO laboratories.

A helium compressor building, anticipated to be slightly larger that at the FTS as a result of increased cryogenic capability, should be located to minimize helium and hydrogen piping to the cryogenic moderator system in the target building.

A new RTBT service building will be sited adjacent to the new proton beam line to the new target building.

A new water tower is expected to be required to achieve the necessary reliability of the new and existing fire protection systems.

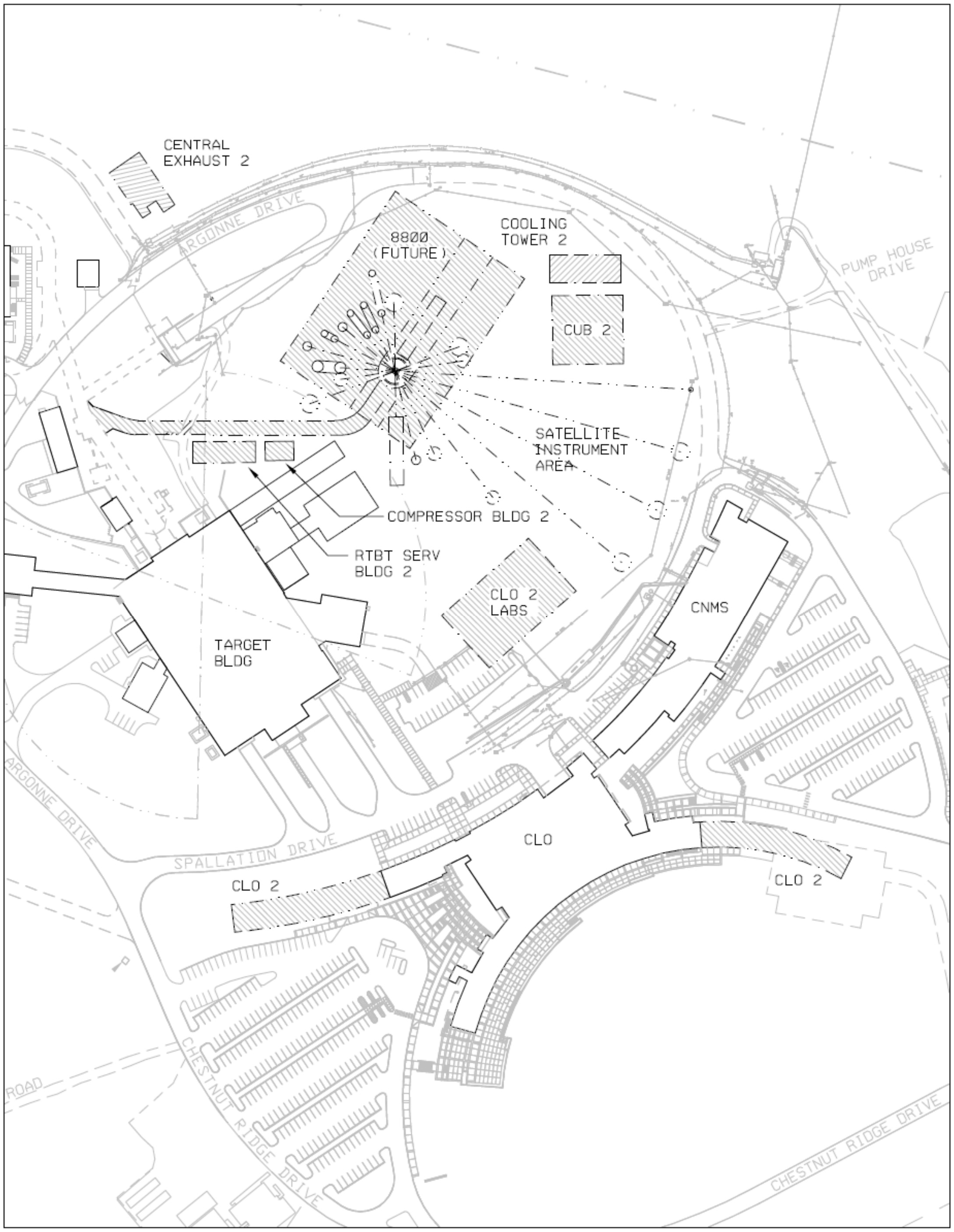

Fig. 3.33. Reference concept layout of the STS. New conventional construction (hatched lines) includes the STS Target Building, Central Lab and Office additions, additional Central Utilities Building, proton beam transport tunnel, and other new utilities and infrastructure. The reference layout of the STS instruments is also shown.

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4.0 FACILITY PERFORMANCE

4.1 SUMMARY OF PERFORMANCE

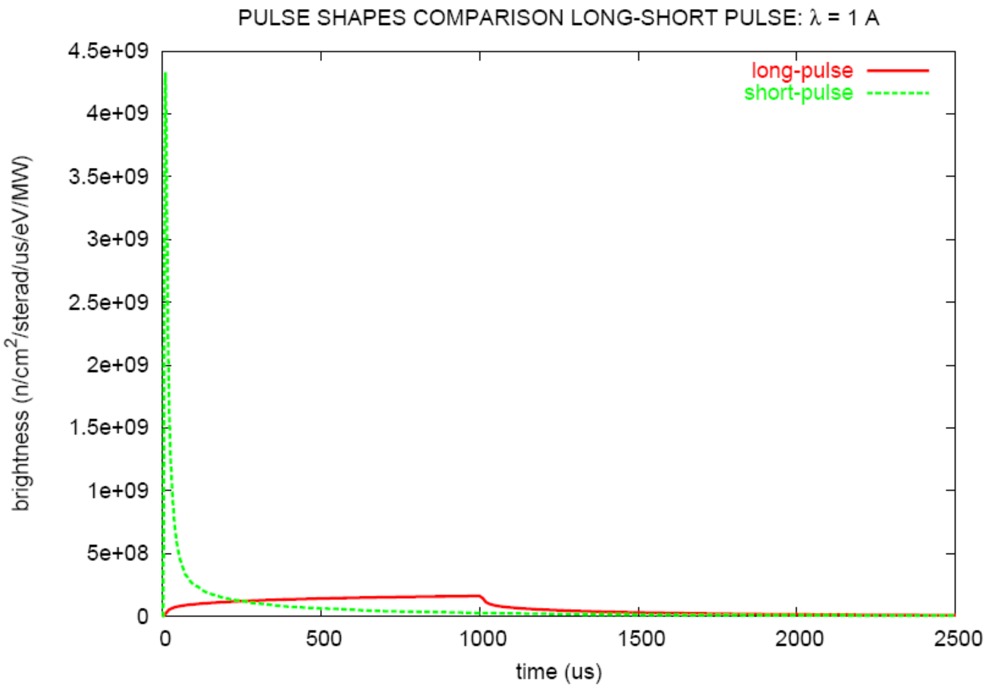
4.1.1 Source Performance

The second target station is optimized to provide a high overall intensity of long-wavelength neutrons. High-intensity long-wavelength neutron beams are achieved by viewing relatively large supercritical para-hydrogen moderators tightly coupled to a liquid-mercury neutron production target. The short-pulse and long-pulse accelerator options, in combination with the moderating behavior of the target/moderator/reflector assembly, determine the neutron pulse shape emitted from the moderator into the beamline. In the short-pulse option, the pulse shape is determined solely by the neutron moderation process. Shorter-wavelength neutrons are emitted in narrower and more peaked pulses, whereas long-wavelength neutrons need longer moderation times, resulting in wider pulses with less pronounced peaking. In the long-pulse option, the pulse shapes are heavily impacted by the proton pulse length, resulting in a time-folding of proton pulse shape and short-pulse neutron pulse shapes.

Figure 4.1 exhibits the fundamental differences of pulse shapes in the short- and long-pulse mode for 1 and 5 Å neutrons, assuming a flat proton pulse profile of 1 ms length for the long-pulse option. Figure 4.2 shows the time-averaged brightness for the STS relative to that at the coupled cold moderator at the FTS, while Fig. 4.3 provides a similar comparison for peak brightness. The time-averaged brightness is the important parameter for instruments that can use the full pulse width (i.e., the full pulse width provides adequate timing resolution), and the peak brightness is the most important parameter for instruments that need to chop the source neutron pulse to provide adequate resolution. Both situations are evident in Fig. 4.4, which summarizes the performances of the reference set of STS instruments. One additional performance difference between the STS and the FTS is that the STS operates at 20 Hz, leaving a much longer period between pulses. This longer period can be utilized to access a larger bandwidth, to provide lower background, or a combination of both. This longer period has also been factored into the instrument performances shown in Fig. 4.4.

4.1.2 Performance for Science - Reference Instrument Performance

Figure 4.4 summarizes the performances of the reference set of instruments on the STS, as detailed in Sect. 3.5 and Table 3.5.3. The improved instrument performance relative to the FTS is a result of both the approximate factor of 5.5 gain in source brightness (Fig. 3.4) and the factor of 3 lower pulse repetition rate that leads to a wider accessible bandwidth. Instruments that can take full advantage of both of these factors thus can perform better than they would at the FTS by a factor of ~16.5. Figure 4.4 shows that this is the case for 70% of the reference suite instruments for the short-proton-pulse mode and for 40% of the instruments in the long-proton-pulse mode (at equal proton beam power to both the FTS and the STS).



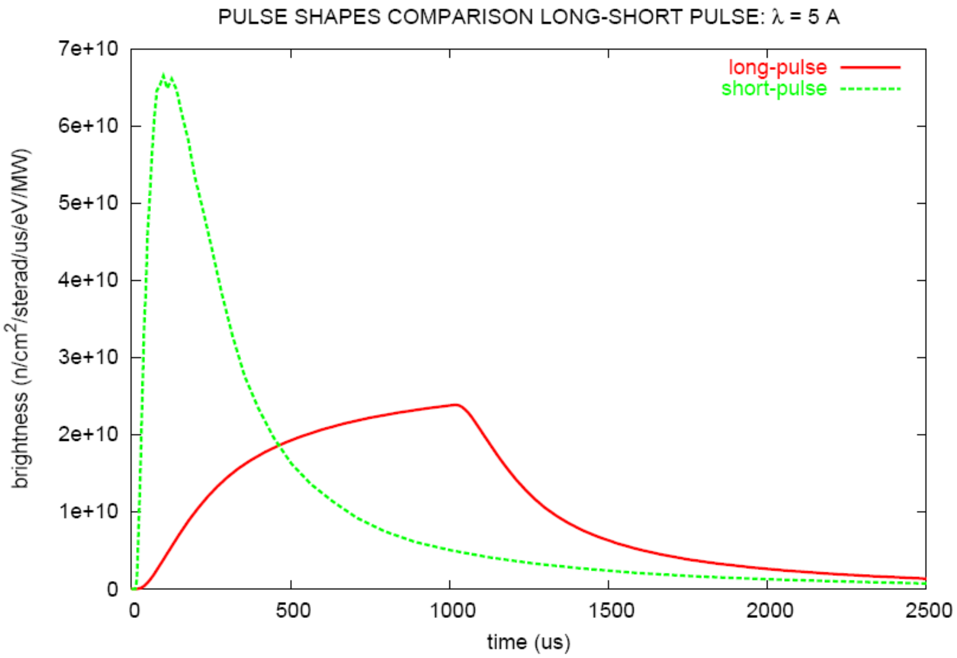


Fig 4.1. Pulse shapes at 1 Å (top) and 5 Å (bottom) for the proposed STS target-moderator system. Pulse shapes are shown for both short-pulse and long-pulse accelerator options. Note that the calculations are based on the same number of protons per pulse for each option.

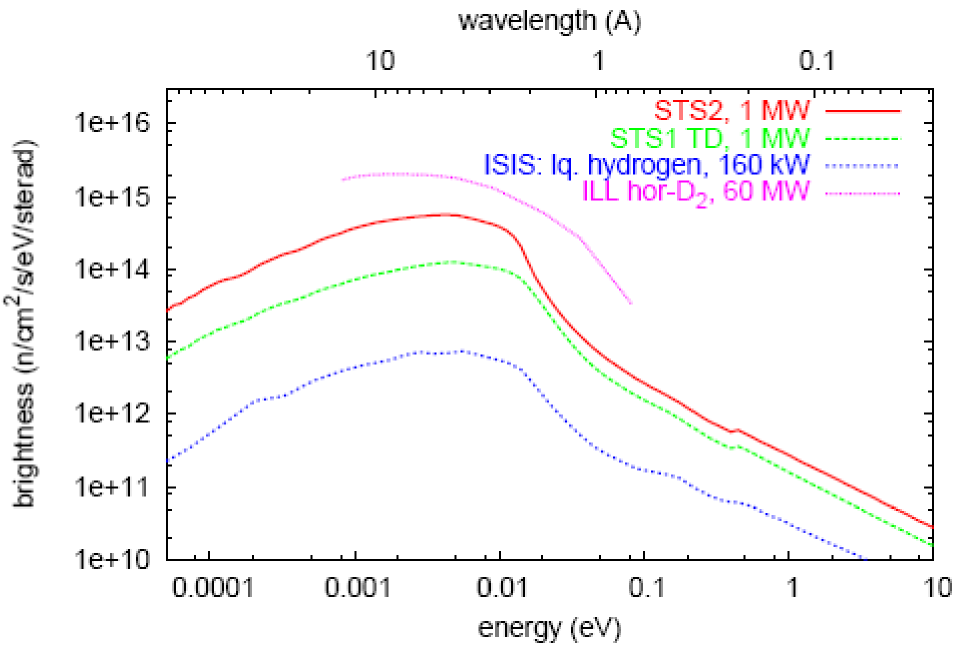


Fig 4.2. Time-averaged moderator brightness calculated for the proposed STS target-moderator system. For comparison, time-averaged cold-neutron brightness is also shown for the FTS coupled cold moderator and for the ISIS pulsed source and the ILL steady-state source.

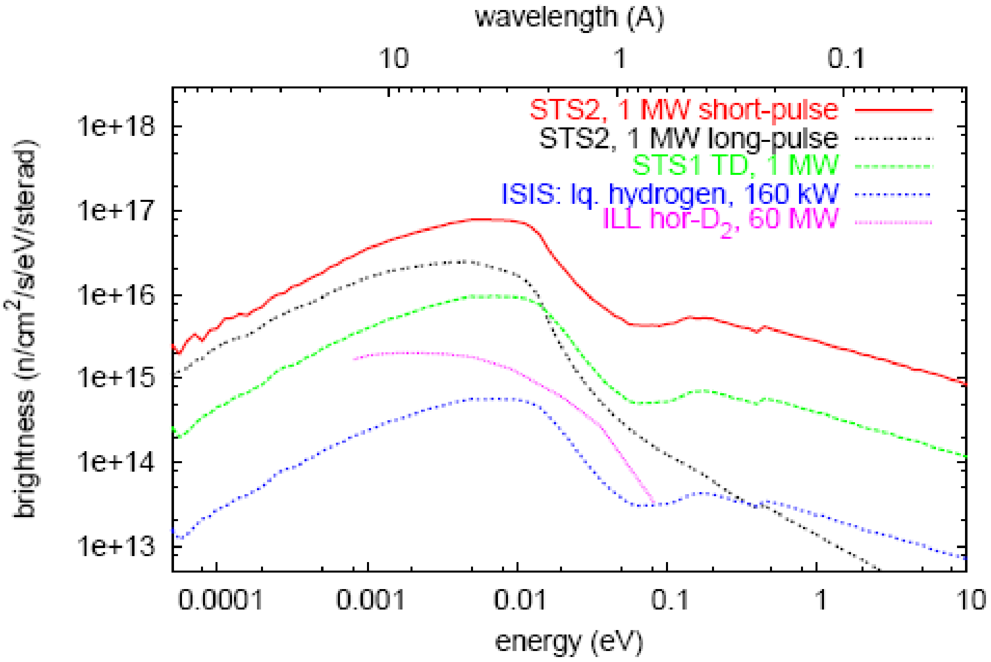


Fig 4.3. Peak moderator brightness calculated for the proposed STS long-pulse target-moderator system. For comparison, peak cold-neutron brightness is also shown for the FTS coupled cold moderator, for an STS with short-proton pulses, and for the ISIS pulsed source and the ILL steady-state source.

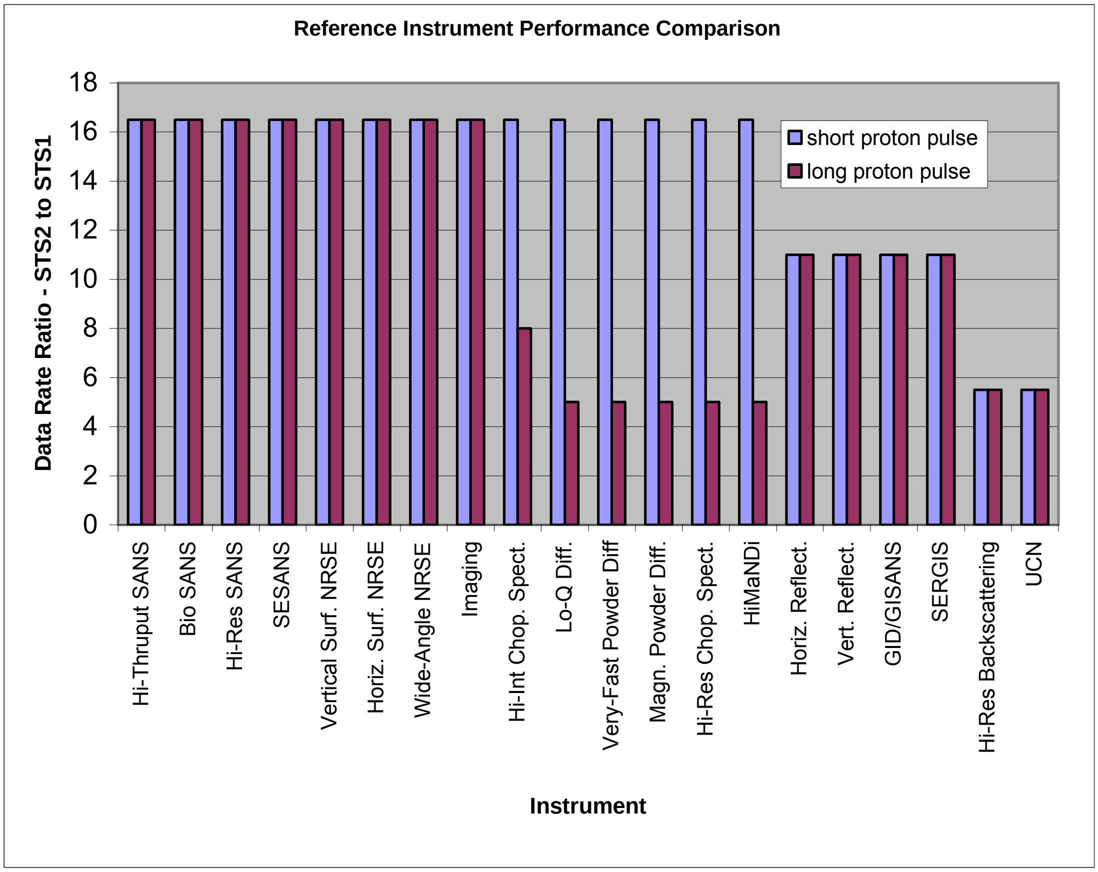


Fig. 4.4. Summary of the STS reference instrument performance—equal time-averaged power case. Data are based on Table 3.5.3. In all cases, the data-rate ratios shown assume the same time-averaged proton beam power for neutron production at the FTS and the STS, and the same time-averaged proton beam power for short- and long-proton-pulse options.

The reference instrument set includes only instruments specifically selected to do well at the STS, and the comparisons in Fig. 4.4 are between the same instrument design at the FTS and the STS. There has been no attempt to make similar comparisons for instrument types best suited to the FTS. In a few cases, the analyses in Chapter 3 also compared the proposed design at the STS with that of a specific planned FTS instrument, and in these cases the STS instrument was shown to have capabilities complementary to those of the FTS instrument.

The data rate ratios from Fig. 4.4 averaged over all 20 reference instruments are 14.3 for the short-proton-pulse case and 11.0 for the long-proton-pulse case. Thus the **STS truly provides an order-of-magnitude gain over the FTS for a broad class of important scientific applications.**

Only 6 of the 20 instruments show significant differences between short-proton-pulse and long-proton-pulse mode. The lowest ratio values occur when the pulse must be chopped to achieve the required wavelength resolution. In that case, the ratios turn out to be approximately the ratio of the peak heights (in accordance with predictions by F. Mezei [F. Mezei, Hahn-Meitner Institute. Personal communication to R. K. Crawford, ORNL, December 2006]). However, as shown in Sect. 3.3, the power readily available to the STS is ~50% more for the long-proton-pulse case than for the short-proton-pulse case. **This extra 50% shifts the conclusions of Fig. 4.4 strongly in favor of the long-proton-pulse option.**

Only very high-level assessments were performed in Sect. 3.5, the source for the data in Fig. 4.4, so the accuracies of the ratio values plotted are not very high. **Nevertheless, the rough magnitudes and trends are quite clear from the figure. The large increases in data rates shown for many of the STS instruments will qualitatively change the types of problems that can be addressed in many forefront areas of science.**

4.1.3 Performance for Science - Potential

The performance of the Reference Instrument Suite at the Reference Concept target station for the STS, as summarized in Section 4.1.2, shows that instruments at this facility could provide more than an order of magnitude increase in data rate for broad areas of forefront science. In several cases these intensities are enough higher that it becomes practical to tighten resolution or to use other techniques to probe previously inaccessible ranges of parameters. For example, analyses of the reflectometer-geometry spin-echo instruments (sections 3.5.4.1 and 3.5.4.2) show that the intense cold neutron beams at the STS will permit tightening the angular resolution to provide an order-of-magnitude extension of neutron scattering dynamical studies to probe such slow motions over longer length scales (up to 1 micron). In another example, these high intensities of cold neutrons will enable the use of GISANS, GID, and SERGIS (sections 3.5.2.3 and 3.5.2.4) to probe lateral structures on surfaces and membranes at length scales from 10 to 1000 nanometers.

Many of the discussions of the Reference Instruments in Chapter 3 made reference to neutron beam focusing devices. At present, neutron focusing devices easily achieve focused beam sizes of < 100 microns. It is reasonable to expect that further improvements in such focusing devices are possible, and that after adequate R&D it will be possible to focus neutron beams to ~10 microns in size [4.1]. The neutron intensity that will be available in such focused beams at the STS will be enough to measure the very weak absorption or scattering produced by the relatively small number of sample atoms illuminated by a beam of this size. This, of course, will permit the study of very small samples of this size. It should also create opportunities to develop instrumentation for various types of scanning neutron probes for exploring minute regions of larger samples. Such devices were not considered as part of the Reference Instrument Suite because these focusing capabilities do not yet exist. Nevertheless, it is likely that instruments of these types will be possible by the time the STS is operational, so this is a very realistic potential performance extension beyond that indicated by the Reference Instrument Suite.

Another potential for extension of the performance beyond that indicated in the reference instrument suite lies in the study of the dynamics of slow motions. The high intensity of cold neutrons at the proposed second target station should make it possible to extend neutron-spin-echo studies of slow motions by an order of magnitude to longer times (up to 10 microseconds) [R. Gaehler, Institute Laue-Langevin. Personal communication to I. S. Anderson, ORNL, September 2007]. However, this will require a significant R&D effort directed at optimizing the spin-echo techniques for this purpose. Similarly, it should be possible to develop sample modulation techniques such as TISANE (time-resolved small angle neutron experiments – see section 6.3.1) to extend kinetic studies down to times as short as 10 microseconds or perhaps even 1 microsecond, thus bridging the gap so that for the first time neutron scattering will be able to span the full dynamical range from picoseconds to minutes.

These quantum jumps in performance made possible by the second target station will lead to qualitatively new scientific capabilities, complementary to those at the first SNS target station. This new facility will extend well beyond current capabilities to be able to answer more difficult questions. These may involve extending measurements to higher resolution, performing the measurements in the presence of a more difficult sample environment and concomitant restrictions to smaller samples, or measurements made to higher precision to look for subtle intensity variations or line shape effects. Many of these more difficult questions involve Grand Challenge scientific problems, as in the study of systems exhibiting greater complexity, such as the complex chemical systems that occur in many soft matter studies, aspects of macromolecular functionality important in biology that can be explored using neutron scattering, or the multi-component systems important to the geophysical properties and functions relevant to earth sciences. The high data rates will also enable routine use of parametric studies to explore another Grand Challenge area, that of systems far from equilibrium and the approach to equilibrium.

4.2 COMPARISON WITH OTHER FACILITIES

Figures 4.2 and 4.3 provide comparisons between the STS (long-pulse baseline case) and the coupled cold moderator at ISIS, which was the world's most intense pulsed neutron source facility until SNS recently surpassed it. These show that **the time-averaged brightness of the long-pulse STS would be roughly two orders of magnitude higher than that of the hydrogen moderator at ISIS and that the STS peak brightness would be nearly two orders of magnitude higher as well**. The ISIS facility has been phenomenally successful in scientific output, but this two-order-of-magnitude jump in available source intensity would enable totally different classes of instruments to address scientific areas far beyond those accessible to the ISIS facility.

Figures 4.2 and 4.3 also provide comparisons between the STS and the most intense cold source at the ILL, the world's premier steady-state neutron source facility for neutron scattering (although intensities at the new cold source at HFIR are comparable to those available at the ILL cold source). Comparisons between source intensities at steady-state sources and those at pulsed sources do not translate directly into relative instrument performances at the two sources. At the pulsed sources, the neutron TOF between production of the pulse and detection of the neutron can be directly related to the wavelength or energy of the neutron. At the steady-state source, other measures to determine the neutron wavelength are required (e.g., monochromator, chopper, velocity-selector); and these other measures lead to less efficient use of the total neutron intensity produced. Comparisons between the two types of sources must be made on an instrument-by-instrument basis, or even better, on the basis of specific scientific problems.

A pulsed source that could produce a time-averaged intensity equal to the time-averaged intensity from the steady-state source would be at least as good as the steady-state source for any neutron beam studies, and better for most. This is not the case for the 1 MW STS in comparison with the ILL, but the STS time-averaged brightness is already within a factor of 3–5 of that at the ILL. Any instrumentation that draws a significant advantage from the source time structure will be able to perform much better at the STS than at ILL. This includes most of the types of measurements for which the STS reference instrument set is optimized.

4.3 REFERENCES

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5.0 SCIENTIFIC EXAMPLES

5.1 SNS SECOND TARGET STATION—A TOOL FOR ADDRESSING "GRAND CHALLENGES" IN CONDENSED MATTER AND MATERIALS SCIENCES

The Committee on CMMP 2010: An Assessment of and Outlook for Condensed-Matter and Materials Physics was recently established by The National Research Council of the National Academies to study the opportunities and challenges in condensed-matter and materials physics (CMMP) in the next decade. This committee published an interim report in September 2006 [5.1] showing its list of eight "Grand Challenges" for CMMP for the coming decade. These eight challenges are listed, along with selected explanatory excerpts from the report. Following each excerpt are a few examples (drawn from the specific scientific studies listed in Sects. 2.1.1–2.1.8) to provide an indication of how a second target station at SNS could help to meet that particular challenge. The examples given, although certainly not exhaustive, indicate the range of such Grand Challenge scientific problems that can be addressed with the SNS second target station and its associated scattering instrumentation.

- **How do complex phenomena emerge from simple ingredients?**

> … *The relationship between the properties of the individual and the behavior of the whole is very subtle and difficult to uncover and lies at the heart of CMMP. The challenge is to understand how collective phenomena emerge, to discover new ones, and to determine which microscopic details are unimportant and which are essential.*

SANS coupled with hydrogen-deuterium isotopic substitution for selective contrast enhancement is an extremely powerful tool for helping to understand the organization of large macromolecular complexes, including understanding the processes by which such organization occurs. The intense long-wavelength beams that would be available at the SNS second target station will be ideally suited to high-throughput SANS instruments that can follow the kinetics and all the intermediate steps in such processes. Such instruments will also be ideal for time-evolution structural studies of self-assembled phases, including systems containing natural or synthetic proteins and nucleic acids with lipids and polymers, and possibly for studying the role of self-assembly in plant growth. Next-generation reflectometers optimized for the cold-neutron beams at the second target station could be used for structural studies of the association and self-assembly of functional clusters in the plane of the membrane.

The combination of high-throughput SANS, long-wavelength diffraction, and reflectometry instruments at the second target station at SNS will also complement the instruments at the first target station to enable structural studies over multiple length scales extending to nanometer dimensions, important for understanding self-assemblies of nanometer-scale building blocks and self-organizing molecular systems. The high-data-rate capabilities of these cold-neutron instruments will also enable kinetic studies over a wide range of time scales to provide a better understanding of the processes involved in such self-assembly.

- **How will we generate power in the future?**

  > *… CMMP is strongly positioned to help address these challenges, which require better fundamental understanding of energy conversion, storage, and transmission, as well as new technologies. … Discovering and understanding new materials will be key …*

For many years neutron scattering has been an important tool for the characterization of new materials and for elucidation of the relationships between the structure and dynamics of the material and the functional properties of interest. Some of the frontier areas will be to use structural, kinetic, or dynamical neutron scattering measurements to provide essential information for optimization of processes and materials in energy storage devices. The high intensity of cold neutrons available at the SNS second target station will enable kinetic studies of faster processes and dynamical studies of slower motions.

Neutron scattering is particularly well suited for monitoring the hydrogen locations and motions in energy storage materials and energy conversion devices. The high intensity of the SNS second target station will allow shorter measuring times, enabling studies of faster processes. These high intensities of cold neutrons will also enable dynamical measurements ranging from the diffusion of dilute ionic species or the relaxation of polymers over a wide time scale to the tracking of the motion of water or other hydrogenous materials during fuel cell operation.

Gas hydrates are currently of considerable interest both as naturally-occurring abundant sources of hydrocarbons and as potential media for sequestration and disposal of greenhouse gases such as CO_2. The high intensity of cold neutrons at the second target station will facilitate accurate determination of the structures of pressure-stabilized gas hydrates and the kinetics of their phase transitions, and in situ structural and dynamical studies of methane clathrates.

Processing of organic fuel stocks and the operation of some fuel cells depend on efficient catalysts. Neutron scattering with the intense cold neutron beams at the second target station will enable much more detailed in situ studies of the structure and operation of complex catalysts, including those based on nanoscale assemblies.

- **What is the physics of life?**

  > *… Researchers are just beginning to see how understanding of materials can be extended to living systems and to recognize the organizing principles that govern living matter. Already, burgeoning understanding is leading to an unprecedented degree of collaboration with biologists, on problems ranging from why proteins misfold and form unwanted structures in diseased tissues, as in Alzheimer's disease, to how the brain works. … a fundamental characteristic of physics, especially CMMP, is its ability to analyze complex systems by identifying their essential and general features. …*

Knowledge of the structure and dynamics of biological macromolecules is essential to the understanding of the functions of these macromolecules at the molecular level. Although general crystal structures of macromolecules are most efficiently found using X-ray diffraction, only neutron diffraction can provide detailed knowledge of the positions of many of the hydrogens, particularly those associated with the functionally important sites in the macromolecule. Such hydrogens frequently play critical roles in the biological activities of macromolecules, so the knowledge provided by neutron diffraction can prove invaluable. The SNS second target station proposed here would significantly extend the U.S. capabilities for such measurements.

Because of their sensitivity to hydrogen (deuterium) and because they enable the use of isotopic substitution for contrast-matching to identify specific structural features, neutrons provide unique capabilities for structural studies of membranes. The intense beams of cold neutrons at the SNS second target station will be ideal for instrumentation that can address the association and self-assembly of functional clusters in the plane of the membrane, the role played by the polymer layer separating the biological membrane from the solid support used for the experiment, and potentially the membrane response to external stimuli such as drugs or pressure, among other things.

The characteristics of the second target station instrumentation will be particularly good for lower-resolution structural measurements using high-intensity SANS with good signal-to-noise capabilities. These instruments, coupled with specific deuteration, will provide information about the positions of individual residues on proteins and multicomponent macromolecular structures in solution; about the protein folding in solution; and about the kinetics, stoichiometry, and organization of large macromolecular complexes.

The high-intensity beams of cold neutrons at the second target station, along with the corresponding neutron scattering spectrometers optimized to study relatively slow motions, will be extremely well suited to dynamical studies of macromolecules. Such studies can probe the conformational flexibility of macromolecules and can be used to verify and/or refine the interatomic potentials used in molecular dynamics simulations of biologically important macromolecules and macromolecular assemblies. Such simulations can help to shed light on the processes that lead to biological functionality. Dynamical studies can also probe the mobility of drugs and nutrients in organs, mobility of nutrients in soils, and denaturation of proteins.

- **What happens far from equilibrium and why?**

> *… [M]uch of the richness of the world around us arises from systems far from equilibrium. Phenomena such as turbulence, earthquakes, fracture, hurricanes, and life itself occur only far from equilibrium. Subjecting materials to conditions far from equilibrium leads to otherwise unattainable properties. … we are just beginning to uncover the basic principles governing such systems. Breakthroughs in this area of CMMP research would affect virtually every discipline in the physical sciences, the life sciences, and engineering.*

Neutron scattering has long been used to study the relaxation of materials toward equilibrium. The more intense beams of cold neutrons that would be available with the SNS second target station would expand the range of relaxation times than can be probed to include both much faster and much slower relaxation processes. The data rates for neutron scattering will be high enough to follow the fast response to external probes and fields (pump-probe experiments). Other areas to be studied include magnetic fluctuations and relaxations, relaxation in glassy materials, and the relaxation of polymers over a wide range of time scales.

- **What new discoveries await us in the nanoworld?**

> *… The potential of nanoscale materials is almost limitless, but we must first overcome two fundamental challenges. The first is physical: how do we control the identity, placement, and function of every important atom in a nanoscale solid, in ways that are practical to apply to real-world materials and devices? The second is conceptual: how do we understand systems that are too large to be handled by brute force calculation, but too small to be tackled by statistical methods? …*

The instrumentation at the SNS second target station, making optimal use of the high-intensity cold neutron beams, will provide unprecedented capabilities for neutron scattering studies of nanoscale materials. These will enable experiments such as dynamical studies of quantum tunneling in molecular magnets and quantum-tunneling-induced gaps in the excitation spectra of magnetic nanoparticles, or structural studies over multiple length scales extending to nanometer dimensions, important for understanding mesoporous materials and self-assemblies of nanometer-scale building blocks. They will also make possible studies of the structure, interactions, and dynamics of complex hybrid materials such as soft-hard nanocomposites and complex polymers in polymer mixtures or blends or in solution.

Nanoscale behavior also introduces fundamental effects in confined systems. The second target station will enable greatly expanded studies of the effects of confinement on phase behavior, thermodynamics, and transport properties of complex liquids, including studies of such liquids in porous material when the sizes of the structural units in the liquids approach nanometer-scale pore sizes.

- **How can we extend the frontiers of measurement and prediction?**

> *The quest to observe, predict, and control the arrangements and motions of the particles that constitute condensed-matter systems is central to the CMMP enterprise. … the experimental, computational, and theoretical tools required to study them are extremely diverse. Many of these tools are developed by individual research groups; other tools, such as synchrotron x-ray and neutron scattering, are developed at large scale national laboratory facilities. Technical innovations that extend the limits of measurement and prediction lie at the forefront of CMMP research. …*

The SNS second target station proposed, with its intense beams of cold neutrons and its suite of optimized state-of-the-art neutron beam instruments, would provide a new set of powerful tools for CMMP research in keeping with this Grand Challenge. This suite of new tools would be ideally suited to address a host of forefront research areas cutting across most of the other Grand Challenges cited in this list.

- **How do we revolutionize the information age?**

> *Extrapolation of Moore's law suggests that, in the next 20 to 30 years, electronic circuit elements will shrink to the size of single atoms. Even before this fundamental limit is reached, electronic circuits will have to operate in a new regime in which quantum mechanics cannot be ignored. … quantum information science envisions computation and communication based not on the familiar laws of classical physics but instead on the often counter-intuitive laws of quantum mechanics. The familiar*

> *binary "bits" of today may tomorrow be replaced by quantum bits or "qubits" capable of encoding vastly more information. CMMP, the science that launched the information age, will play a pivotal role in determining its future.*

Quantum phenomena and the behavior of materials at the nanoscale are important forefront areas in the information age. Instruments on the intense cold neutron beams at the SNS second target station will facilitate a wide variety of research in the dynamics of thin films, wires, and dots. The high neutron intensities will permit the use of smaller sampling volumes to probe local regions of bilayers or biomolecular or polymeric ultrathin microelectronics and photonics films in situ.

Magnetic storage devices will continue to play important roles, at least in the near future. The neutron instrumentation at the second target station will provide new capabilities for the study of lateral magnetic structures on thin films, magnetic domain wall structure and dynamics, quantum tunneling in molecular magnets and magnetic nanoparticles, and spin-density distributions and waves in organic materials. Such studies should lead to better understanding of magnetic storage devices, including understanding of the effects of spin structures and fluctuations.

- **How can we inspire and teach others?**

> *... Many of us benefit from the torrent of new and improved electronic devices, but few are aware that these products are the fruits of a rich and coherent scientific discipline characterized by an inseparable mix of fundamental and applied research. Limited public awareness and understanding of science present an increasing danger to our nation's economic security and are most dramatically reflected in the current crisis in primary and secondary school science education. ... It is critical that we infuse a new generation of scientists with the knowledge, skills, creativity, versatility, and sense of wonder needed to meet the challenges ahead.*

The SNS itself is intended primarily as a world-class research facility rather than as a teaching facility, and this would also be the case for a second target station at the SNS. However, the availability of two such major best-in-the-world facilities in the United States would send a very strong message about the continued excitement in the pursuit of fundamental and applied knowledge across the wide range of CMMP, and the national importance placed on this pursuit. Both of these world-class facilities will be of major importance in attracting and educating the next generations of scientists in a broad range of forefront scientific disciplines.

5.2 SPECIFIC EXAMPLES

This section provides in greater detail a few examples illustrating the breadth of forefront scientific problems that could be addressed only with the types of capabilities to be made available with the SNS second target station.

5.2.1 Superconductivity Studies at the Second Target Station

5.2.1.1 Introduction

Superconductivity is the amazing ability of materials to conduct electricity with no loss. Such a phenomena is well understood for materials with superconducting transition temperatures (Tc) near the absolute zero of temperature (−273°C). However, a revolution took place around 20 years ago when entirely new families of superconductors based on the cuprate oxides were discovered. These work at much higher temperatures, with the high-temperature superconductor $HgBa_2Ca_2Cu_3O_8$ being the record holder. It operates at temperatures as high as 164 K (−109°C). The layered structure of this complex oxide allows the electrical current to travel easily along certain crystal planes, leading to superconductivity at these remarkably high temperatures.

No real understanding of the mechanism permitting superconductivity at these high temperatures has been developed, and one of the Grand Challenges listed in *Science* magazine is *What is the pairing mechanism behind high-temperature superconductivity?* Electrons in superconductors move together in pairs, and after two decades of intense study, no one knows what holds them together in the complex, high-temperature materials.

As an energy carrier, electricity has no rival with regard to its environmental cleanliness, flexibility in interfacing with multiple production sources and end uses, and efficiency of delivery. In fact, the electric power grid was named “the greatest engineering achievement of the 20th century” by the National Academy of Engineering. However, the growing demand for electricity will soon challenge the grid beyond its capability, compromising its reliability through voltage fluctuations that crash digital electronics, and brownouts that disable industrial processes and destroy electrical equipment. The American blackout of 2003 affected 50 million people and caused approximately $6 billion in economic damage.

Superconductivity offers powerful new opportunities for restoring the reliability of the power grid and increasing its capacity and efficiency. Superconductors are capable of carrying current without loss, making the parts of the grid they replace dramatically more efficient. Superconducting wires carry up to five times the current carried by copper wires that have the same cross section, thereby providing ample capacity for future expansion while requiring no increase in the number of overhead access lines or underground conduits. Their use is especially attractive in urban areas, where replacing copper with superconductors in power-saturated underground conduits avoids expensive new underground construction.

Superconducting transformers cut the volume, weight, and losses of conventional transformers by a factor of two and do not require the contaminating and flammable transformer oils that violate urban safety codes. Unlike traditional grid technology, superconducting fault current limiters are smart. They increase their resistance abruptly in response to overcurrents from faults in the system, thus limiting the overcurrents and protecting the grid from damage. They react fast in both triggering and automatically resetting after the overload is cleared, providing a new, self-healing feature that enhances grid reliability. Superconducting reactive power regulators further enhance reliability by instantaneously adjusting reactive power for maximum efficiency and stability in a compact and economical package that is easily sited in urban grids. Not only do superconducting motors and generators cut losses, weight, and volume by a factor of two but they are also much more tolerant of voltage sag, frequency instabilities, and reactive power fluctuations than their conventional counterparts.

The challenge facing the electricity grid to provide abundant, reliable power will soon grow to crisis proportions. Incremental advances in existing grid technology are not capable of solving the urban power bottleneck. Revolutionary new solutions are needed, such as like the kind that come only from superconductivity. Unfortunately, present-day superconductors have rather low current carrying capability; and although the remarkable increase in transition temperatures has make a huge impact, higher transition temperatures are very desirable.

Two major research directions need to be taken. The first is the discovery of materials that have better properties; the second is the development of a theoretical understanding of the forces that permit electron pairing at higher temperatures. The cuprates are characterized by particularly strong interactions between the electrons, leading to new physical effects. It appears that, in some metals, such "free particles" simply do not exist; so the collective behavior of the electrons has to be considered in its full complexity, resulting in qualitatively different transport and magnetic properties.

New phases of matter can arise, and novel effects often emerge near the associated phase boundaries. Understanding the behavior of such "strange metals" is one of the most important challenges the materials community is facing now.

5.2.1.2 New materials

There are no simple and straightforward directions as to how to create new classes of superconductors. All families of superconductors known to date were discovered serendipitously. However, this does not need to be the case in the future, and we can point out some likely possibilities where breakthroughs could occur. We now know that a large energy scale can sometimes be translated into a high critical temperature. This is an important ingredient. A few possibilities for creating a superconducting state are (a) lattice vibrations (with the negative electrons being attracted to the positive ions), (b) spin fluctuations (where pairs are bound because of magnetic interactions between the electrons' spins), and (c) valence fluctuations (where local valence changes on an ion attract two electrons to form a pair). This list can be continued, and it is important in our search for novel superconductors to cast the net broadly enough to be able to capture wide classes of materials and mechanisms. Figure 5.1 shows the crystal structure of the first high-T_c superconductor, $La_{2-x}Sr_xCuO_4$ with a T_c of ~40 K, versus the record holder, $Hg_{0.2}Tl_{0.8}Ca_2Ba_2Cu_3O_8$ with a T_c of ~140 K .

The discovery of superconductivity in layered copper oxide (CuO_2) compounds was remarkable, not only because of the high temperatures at which superconductivity survives but especially because these materials had been thought to be poor electronic conductors. The key components of these materials are the CuO_2 planes. Inorganic chemists have found a wide variety of spacer layers that can be inserted between the CuO_2 planes, resulting in a considerable number of different cuprate compounds that exhibit high-temperature superconductivity. For a given compound, the electronic properties of the CuO_2, especially the superconductivity, can be tuned by adjusting the in-plane charge density. The latter is typically achieved by chemical substitution ("doping") or by alteration of the concentration of oxygen atoms in the spacer layers. Over the past two decades, considerable effort has gone into mapping out the electronic properties of layered cuprates as a function of in-plane charge density and temperature.In conventional superconductors, such as lead and niobium, one can also alter the superconducting critical transition temperature, T_c, by chemical substitution; however, the phase diagrams of such materials are relatively simple. The normal (nonsuperconducting) state at

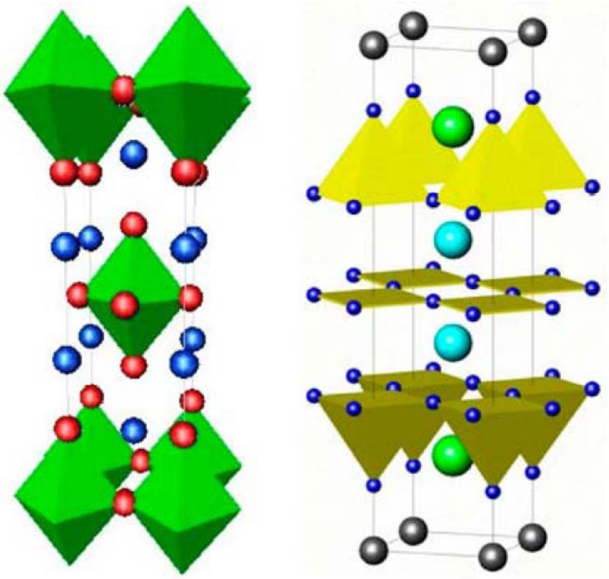

Fig. 5.1 Crystal structures of high-T_c superconductors. $La_{2-x}Sr_xCuO_4$ (left) compared with the high-T_c record holder, $Hg_{0.2}Tl_{0.8}Ca_2Ba_2Cu_3O_8$ (right) with a T_c of ~140 K. [5.2] (*Source*: *Basic Research Needs for Superconductivity, Report of the Basic Energy Sciences Workshop on Superconductivity*, May 8–11, 2006, www.sc.doe.gov/bes/reports/files/SC_rpt.pdf).

$T > T_c$ is generally a good electronic conductor. Chemical substitution can alter the density of conduction electrons, resulting in shifts in T_c, but no other electronic phases of matter appear. As discussed below, the typical phase diagram of a cuprate compound is quite different. By tuning the charge density, onecan change from a good electronic conductor to an electronically insulating phase. Magnetically ordered and disordered phases are prominent, and unusual charge-ordered phases have been discovered. Some of these various types of electronic order appear to compete with the superconductivity. Of course, the proximity in the phase diagram of superconductivity to an alternative type of electronic order could result from closely related interactions. Thus the study of "competing" order may yield important clues for understanding the mechanism of superconductivity, perhaps even providing approaches to manipulating the superconducting state.

The materials problems for the understanding of the new superconductors are thus becoming increasingly complex. This complexity may show up structurally as very large unit cells, phase coexistence, subtle superlattices and distortions, and additional length scales that must be considered. To handle these structural problems, scientists need single-crystal and powder diffractometers optimized for both excellent resolution ($\Delta d/d$) and low background. Full exploitation of these scientific topics requires greater intensity and/or range and resolution capabilities not available with instrumentation at a single target station. Requirements include one or more single crystal diffractometers, a high-resolution powder diffractometer with $\delta d/d$ down to 0.1%, and a high-intensity powder diffractometer with somewhat lower resolution. The suite of powder diffractometers must be capable of spanning the range $0.3 \leq Q \leq 12$ Å^{-1} and at least some of them must be capable of measurements with polarized neutrons and high magnetic fields. The high intensities of long-wavelength neutrons available at the SNS second target station will make possible instruments that complement and extend the capabilities available at the first SNS target station. Both sets of instrumentation are needed to optimally span this range of requirements.

The most direct approach to finding new superconductors is to identify and execute a series of systematic searches of phase space to find new compounds. These can be conducted by identifying promising regions of composition space and rapidly examining as many compounds as possible in this space. Such studies are what yielded the explosion of intermetallic superconductors in the 1950s and 1960s. These need to be resumed in ternary or higher space, focusing on likely regions, e.g. ternaries with light elements.

Often, the most interesting new superconductors are difficult to make because of either the complexity of the chemistry or structure or more mundane materials issues. Progress in experimental study and theoretical understanding has been hampered by materials problems ranging from large unit cells to stoichiometry problems caused by the volatility and reactivity of constituent elements. Better material and sample quality is the critical prerequisite for rigorous experimental work where the physics is in the "clean limit"—free of any spurious, extrinsic effects. Furthermore, improvement in physical properties—for example T_c, H_{c2}, J_c—brings known superconductors closer to possible applications. In the absence of large single crystals, high-quality polycrystalline samples are valuable for characterizing superconducting properties and often define the basic features like the transition temperature, condensation energy, grain boundary connectivity, and electron and phonon density of states. The considerably more challenging synthesis of single crystals makes high-quality polycrystalline samples the first target for exploring the behavior of newly discovered superconductors.

5.2.1.3 Vortex matter

The behavior of superconducting vortex matter determines how a superconductor's current-carrying capability affects its suitability for technological applications. The study of vortex matter spans the broad spectrum from discovery science through use-inspired basic research to applications. Beyond its fundamental impact on all practical applications of superconductivity, its theoretical concepts touch upon the subjects of cracks and dislocations in solids, the dynamics of domains in magnets, and the physics of localized electrons in metals. The discovery of high-temperature superconductors dramatically broadened the range of the temperatures and magnetic fields considered in studying vortex matter and introduced qualitatively new static and dynamic features into its behavior. Since that discovery, remarkable progress has been made in our understanding of vortex matter. We have observed the melting of an ordered array of vortices (vortex lattice) into a novel vortex liquid phase. We continue to search for means to "dam" or "pin" the flow of the vortex liquid, a necessary condition for achieving zero resistance.

The vortex lattice can be seen directly by SANS, as shown in Fig. 5.2. The vortex lattice disappears as the magnetic field or the temperature increases. This gives the upper range of use for the material for current transport. Long-wavelength neutrons are needed for measurement, as the length scale of the vortex lattice is quite long. Quite often only small samples are available, as single crystals are needed for these studies. Therefore, high-performance small angle spectrometers are required, making the intense beams of long-wavelength neutrons at the SNS second target station ideal for these measurements

5.2.1.4 Excitations in superconductors

It was mentioned earlier that likely possibilities for creating a superconducting state are lattice vibrations and spin fluctuations (in which pairs are bound because of the electron attraction to the positive ions in the case of phonons and between spins in the magnetic case). The magnetic interaction is a popular choice since the parent compounds are insulating antiferromagnets with superconductivity achieved by doping with either electrons or holes. The phase diagram has been determined in a large part by neutron scattering.

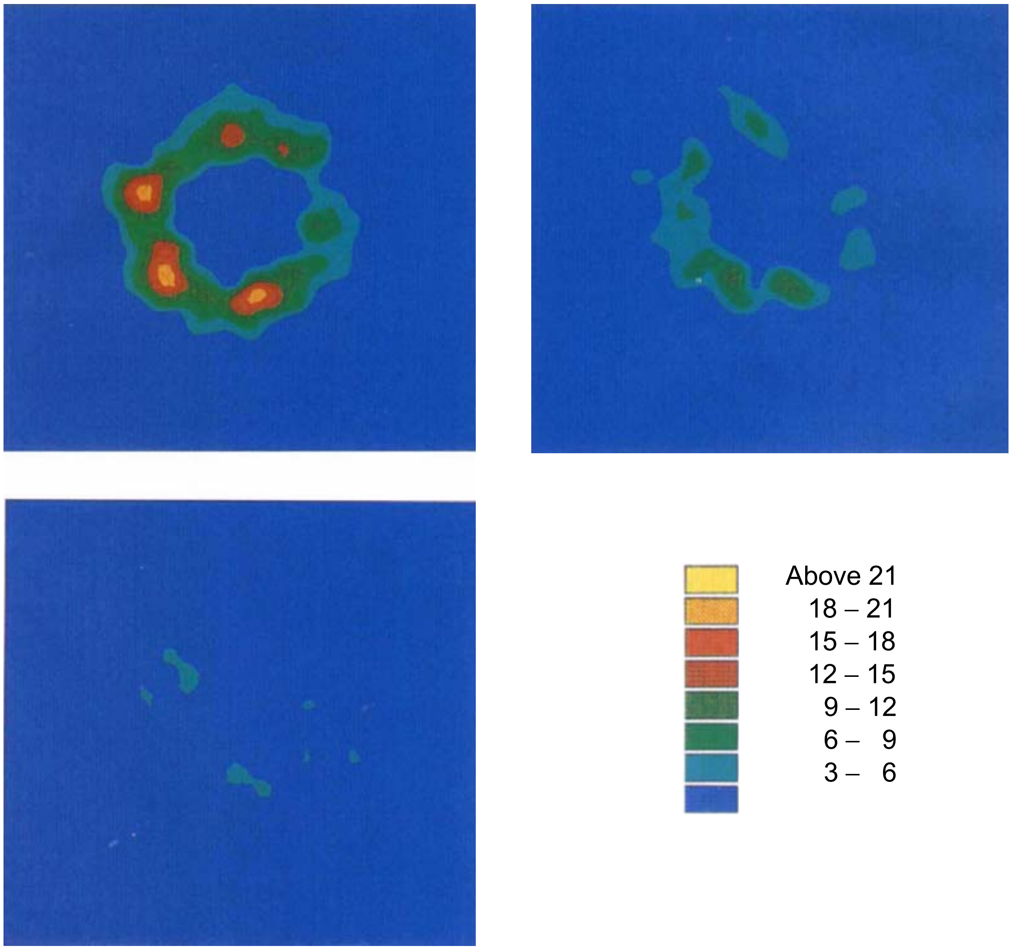

Fig. 5.2. Small-angle neutron scattering pattern from the vortex lattice. The vortex lattice disappears as the magnetic field is made larger for the high-temperature superconductor BSSCO (R. Cubitt et al., *Nature* **365**, 407, 1993).

The hope is that the extent and the nature of the magnetic state can be established by neutron inelastic scattering and the superconductivity calculated for a series of materials with different doping. This procedure is under way, but much needs to be done.

Figure 5.3 shows the magnetic excitation spectra for $YBa_2Cu_3O_{6.6}$ measured with a neutron spectrometer. It is found at low energies that the scattering is incommensurate with four spots. As the energy is raised, the scattering narrows to a single commensurate peak called the “resonance.” Finally, at high energies, four spots are again found but are rotated by 45° from the low-energy spots. The pattern is complex, so much work is needed to see if such a pattern can account for the

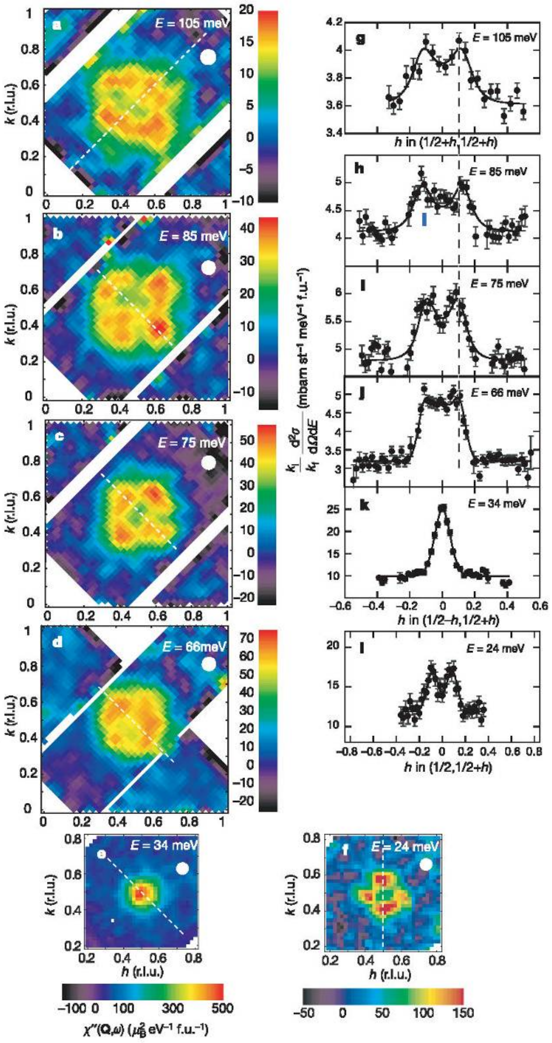

Fig. 5.3 Magnetic excitation spectra for YBa$_2$Cu$_3$O$_{6.6}$. Measurements made with the MAPS spectrometer at the ISIS neutron source at the Rutherford Appleton Laboratory in the UK. (S. M. Hayden, et al., *Nature* **429**, 531–534, 2004).

superconductivity. Measurements of this pattern need to be extended to both lower and higher energies. This requires chopper spectrometers with cold neutrons, thermal neutrons, and high-energy neutrons. High resolution is also needed, as the pattern of magnetic scattering is detailed with considerable fine structure. As materials are investigated with higher hole doping and higher T$_c$ values, the scattering gets weaker and more difficult to observe. Thus the unprecedented high intensities to be provided by the SNS second target station will be essential in the quest to complete this picture and further the understanding of the fundamental basis of high-temperature superconductivity. Many measurements will be needed before the magnetic excitations are sufficiently well characterized to reveal whether they can account for the energy needed to establish superconductivity.

The phonon excitations show changes in the cuprate superconductors as the temperature is changed. It is generally thought that these phonons cannot account for superconductivity in the same way as they do for conventional low-temperature superconductivity. However, the phonons may play a role in a different manner or combine with the magnetic excitations to produce the electron coupling needed for superconductivity. Chopper spectrometers with high intensity are needed to determine the phonon excitations. High resolution is needed as the phonon branches are complicated and are near together in energy. Very high resolution is needed to measure phonon lifetimes, which can give a direct measure of the electron coupling. In this case, spin precession or back-scattering spectrometers are needed to measure the phonon widths in energy. The intensities and instrumentation available at the second target station will be crucial for success in many of these measurements.

Figure 5.4 shows the difference in the intensity of the high-energy oxygen phonon modes in $YBa_2Cu_3O_{6.95}$ at high and low temperatures. The phonon modes were measured with inelastic neutron scattering on the MAPS spectrometer and shift considerably with temperature, but it is not clear how this is related to superconductivity. Higher resolution and intensity would give a much clearer picture of the phonon shifts and how they might couple to superconductivity.

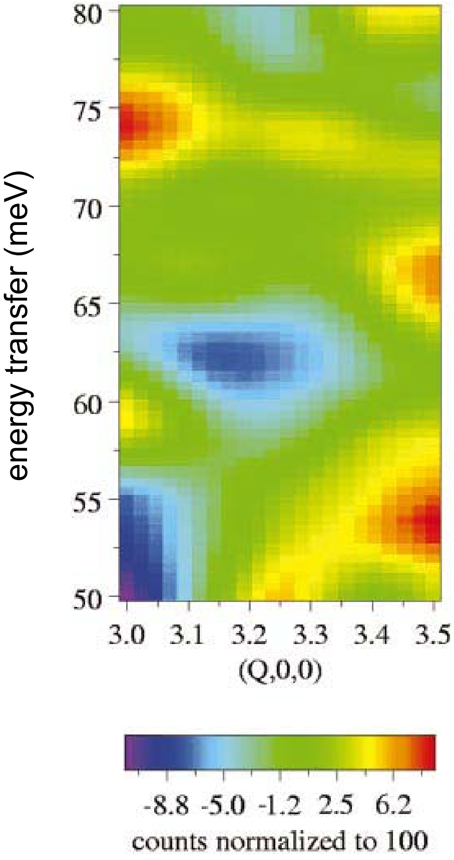

Fig. 5.4 Difference in intensity of the high-energy oxygen phonon modes in $YBa_2Cu_3O_{6.95}$ between high and low temperatures (J.-H. Chung et al., *Phys. Rev. B* **67**, 014517, 920030, 2003).

It is clear that neutrons will play a major role in the discovery of new and better superconductors and in the Grand Challenge of understanding the origin of the superconductivity in high-T_c materials, and it is clear that the SNS second target station has much to offer in this area. A wide range of neutron spectrometers is needed to examine the many issues involved. However, the benefits that better superconductors would bring are well worth the effort.

5.2.2 Neutron Studies of Soft Matter at the Second Target Station

The field described as soft condensed matter physics encompasses a wide range of materials and materials problems. In each case, the materials are composed of long-chain molecular materials with complex short- and long-range interactions. In these materials, both entropic and enthalpic interactions are important. Among this class of materials are polymers, proteins, surfactants, and liquid crystals. Although the complexity of the intra- and inter-molecular interactions in these materials makes them challenging to understand, this complexity yields a rich variety of materials properties that can be altered by tuning the interactions. The nature of these materials lends them to uses such as friction modification in cookware and engine lubricants, lightweight high-strength composite materials, and self-assembled scaffolds for forming nanostructures. Complex biomaterials such as proteins and DNA are also examples of soft matter, with their complex dynamic and structural interactions within living cells.

Neutron scattering has been a valuable tool for studying soft matter in all of the systems noted. The reason for the success of techniques such as SANS, neutron reflectometry, and NSE, for example, is selective deuteration. Individual sub-units can be highlighted for studies of the structure and dynamics of individual molecules in a matrix or of the collective structure or dynamics of particular molecular segments. Nevertheless, using existing neutron sources, many of the properties of soft matter remain just outside experimental reach because of flux limitations. With the advent of the gains afforded by the STS, these studies can be expanded to include smaller sample volumes or areas, greater Q-ranges for improved measurements over larger length scales, and dynamic studies on expanded time scales. This will afford researchers new tools to study the structure and dynamics of soft materials .

Many problems in soft condensed matter that can be addressed using the STS are related to the Grand Challenges in Physics stated in Sect. 5.1. However, they are too numerous to list here. Instead, we present a few problems in the areas of surfaces and interfaces that illustrate a small part of what may be studied with neutrons using neutron reflectometry and SANS.

5.2.2.1 Soft matter in confined geometry

Polymer molecules at solid or fluid interfaces have an enormous spectrum of applications and functions in a wide variety of technologies. For example, they provide a mechanism by which to impart steric stabilization of colloidal dispersions, are used as protective coatings (including providing mechanical protection of solids against friction and wear), and are used to modulate dispersion properties (such as rheology) under a variety of processing conditions [5.3]. They can be designed either to promote adhesion (e.g., epoxies and glues) or to prevent sticking (e.g., Teflon coating for metal surfaces). In the same manner, proteins, which are natural biopolymers, govern the interactions between and functions of biological cell surfaces.

Knowledge of the conformations that adsorbed or terminally anchored chain molecules adopt when subjected to confinement and solvent flow is essential for predicting the interaction forces and tribological and rheological properties in thin-film technologies [5.4]. Theoretical [5.4] and modeling [5.5, 5.6, 5.7] investigations have been performed on polymers chemically or physically tethered to surfaces. When densely packed polymers attached to a substrate are placed in a good solvent (for the unbound end of the polymer), the polymer free energy consists of a competition between the osmotic forces that want the chains to dissolve in solution and the energy cost of stretching the coiled chain. The resulting carpet-like molecular structure is referred to as a "polymer brush." One of the characteristic properties calculated for these systems is the polymer segment density profile normal to the surface.

Recent work has been reported on a confinement cell used in neutron reflectometry experiments [5.8]. The heart of the cell consists of two highly polished single-crystal blocks (silicon, quartz, sapphire) that can be coated with polymers, for example. These blocks can then be placed face to face and lightly pressed to form a uniform, flat, gap as small as 1000 Å between the two surfaces. With this geometry, neutron reflectivity experiments can be performed to examine the structure of the polymer confined between the single-crystal surfaces (Fig. 5.5).

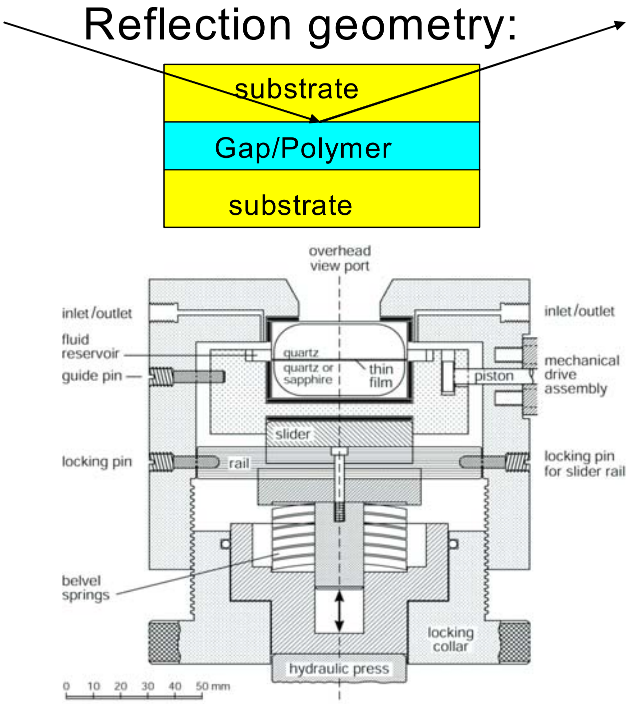

Fig. 5.5. Schematic diagram of a confinement cell used for neutron scattering (*Source*: ref. 5.7).

With present neutron sources, the area of the film confined between the crystals must be ~10 cm^2 in order to obtain a sufficiently large reflectivity signal. This area limits the gap spacing between the crystals owing to the waviness of the surfaces to ~1000 Å. In recent work [5.9], it was shown that the use of X-ray reflectivity gaps of as small as 15 Å is possible over areas of ~0.02 cm^2. With the advent of the second target station, available fluxes will be an order of magnitude higher than at present sources (10 × FTS). This level of flux will allow researchers to reduce the needed area for a confinement cell to 1.0 cm^2 or less so that the gap for neutron reflectivity experiments can be reduced to ~100 Å.

This length scale for confinement opens up several new areas of study, particularly studying the area of interactions between lipid membranes. Phospholipid bilayer membranes supply the basic scaffold for the living cell membrane. Typical bilayer thicknesses are on the order of 50 Å. Thus coating the two opposing surfaces with single-bilayer membranes enables researchers to study the effects of the confinement on the two films. By attaching proteins to or inserting them into the bilayer surfaces, researchers can study the effects as two cells on the protein approach each other. These data will yield for the first time structural data complementary to the intermolecular forces obtained using the Surface Forces Apparatus [5.10] on these important materials.

5.2.2.2 TOF SANS studies of the dehydrogenation kinetics of ammonia borane complexes in solution for hydrogen storage

Amine borane (AB) complexes with the empirical formula $B_XN_XH_X$ have great potential as high-capacity hydrogen storage materials. Amonia borane (BH_3NH_3), is the simplest of the AB complexes, having material hydrogen content of 19.6 wt % and a volumetric energy density of ~4.94 kWh/L, far surpassing that of liquid hydrogen (2.36 kWh/L) [5.11]. It is currently considered to be one of the most promising hydrogen storage materials that have the potential to meet DOE's near- and long-term hydrogen storage targets. Hydrogen gas can be released from ammonia borane by heating (a process called thermolysis). This process begins at temperatures of ~105°C; however, to discharge a substantial amount of hydrogen, temperatures of above 500°C are needed. The amount of energy required for dehydrogenation may prevent widespread use of AB complexes in future transportation applications; therefore, new energy-conserving routes to dehydrogenation are needed to make effective use of ABs.

Solid-state dehydrogenation of AB complexes below 80°C results in negligible hydrogen production; however, recent studies have shown that adding small amounts of various solvents may facilitate the dehydrogenation at low temperatures (see Fig. 5.6). The reasons for the variable efficiency of different solvents are currently not understood. However, it was recently suggested [5.12] that the variations in efficiency may be related to the influence of solvent quality on the kinetics of AB polymerization in solutions at early stages of dehydrogenation (<10 min). Structural changes induced by dehydrogenation in solutions of AB complexes may be explored using SANS, which is the premier technique for establishing the structure-property relationships in polymer solutions on a relevant scale of 1–100 nm [5.11]. TOF SANS is especially suitable for the investigation of kinetic processes in soft matter. High-flux TOF SANS machines built at the SNS second target station will allow investigation of the fast kinetics of the structural changes (sequences of transient polymeric structures) in polymerized AB complexes at the initial stages of dehydrogenation processes in various solvents, in addition to static time-averaged conformation (equilibrium structures) of the formed polymers. Availability of high-flux TOF SANS instruments will enable exploration of the time dependence of the overall polymer structure in solution, including insights into the reproducibility (stability) of a given configuration through abrupt changes in state variables such as temperature and/or pressure.

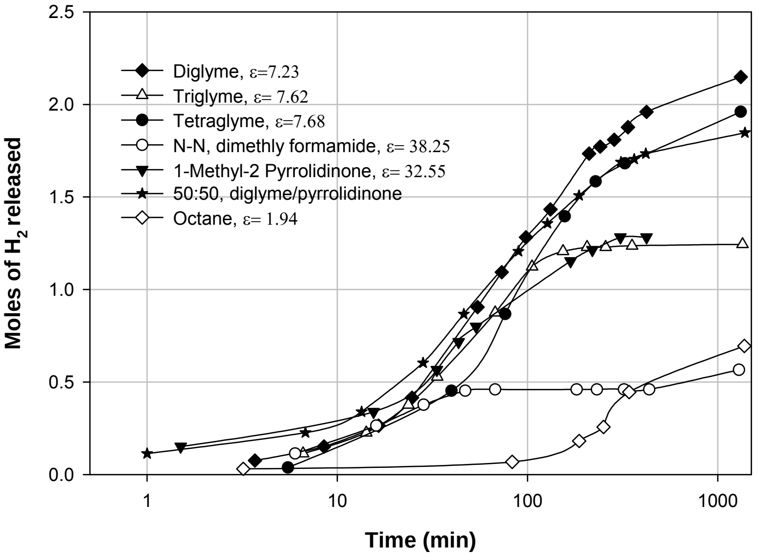

Figure 5.6. Hydrogen evolution vs time during thermolytic dehydrogenation. Studies of AB complex (approximately 0.2 g) using 0.4 mL of various solvents at 70°C. (N. Mohajeri, Florida Solar Energy Center. Personal communication with G. S. Smith, ORNL).

5.2.2.3 Lipid membrane structure—rafts and proteins

Cell membranes consist of bilayer leaflets of mixed lipids, proteins, glycolipids, and other cellular components. The lipids form the basic membrane with a head-tail-tail-head arrangement in which the head groups are hydrophilic and the tails are hydrophobic. Details of how the cell membrane performs many of its functions are still unknown. For example, when the cell brings material (e.g., proteins) into its interior, it may do so by engulfing the material by budding off part of the cell membrane. During this operation, called endocytosis, the membrane must locally change shape from a flat bilayer to a highly curved vesicle [5.13]. What drives this local change of curvature is not well understood.

One of the more novel ideas regarding the function of lipid membranes is that the membrane itself drives some of the functions as opposed to being a passive scaffold. One way lipids can regulate how proteins interact with the cell membrane is through the formation of lipid rafts [5.13, 5.14]. Most of the lipids in the cell membrane are in an L_α phase in which the hydrophobic tails are in a disordered state; this arrangement exhibits no long-range order within the plane of the bilayer. However, it is postulated that there are small domains of lipids with ordered tails [5.15]. These small domains are called "rafts." Rafts have been observed in model bilayer systems consisting of sphyngomylein, cholesterol, and water; but it is not certain if they exist in the more complicated cell membranes [5.15]. The domains interact and bind with water-soluble proteins differently from liquid-phase lipids. It has even been shown that the lipid bilayer can regulate the functions of transmembrane proteins such as ion channels [5.16], since a channel in a raft feels a compressive force different from that in the disordered lipids (Fig. 5.7).

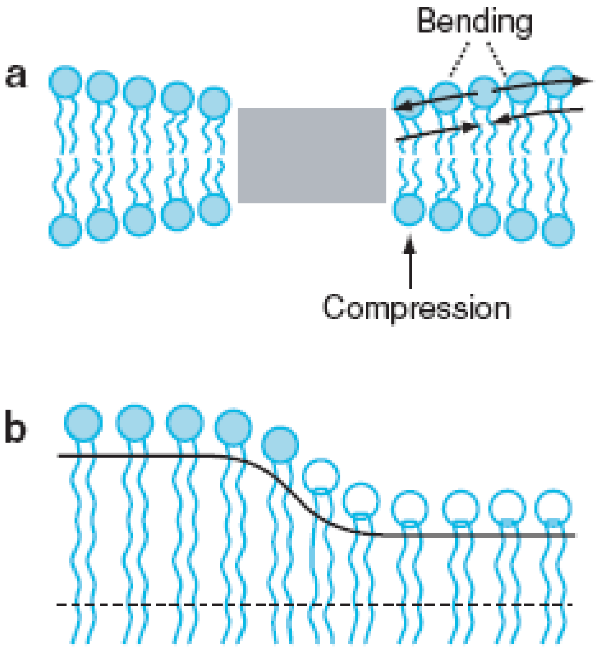

Fig. 5.7. Bilayer deformation. Schematic drawings illustrating bilayer deformation (a) adjacent to a transmembrane protein (gray rectangle) and (b) at the boundary between a thick raft bilayer (blue headgroups) and a thinner non-raft bilayer (white headgroups). ([*Source*: ref. 5.14])

The lateral phase separation and structure in lipid bilayer membranes, therefore, play an important role in the function of living cells. Similarly, the function and in-plane structure of membrane proteins are also related to cell function and to the arrangement of rafts and other in-plane variations. Until now, few studies have been done using neutrons or even X-rays to directly measure the in-plane structures of these materials. The lack of studies is due to the difficulty in studying bilayers in an aqueous environment with X-rays and to the low fluxes for neutrons. With the advent of the surface-sensitive spectrometers (GID, GISANS, and SERGIS; see Sect. 3.5) at the STS, new studies of multi-bilayer and potentially single-bilayer systems can be accomplished. The lipids, cholesterol, and proteins for the model systems studied can be deuterated to provide the in-plane contrast not afforded to X-ray scattering. In this way, the domain sizes can be studied using the GISANS and SERGIS instruments, and the in-plane structure can be examined using GID. Coupling these techniques with reflectometry, a more detailed picture of the structure-function relationships of these complex systems can be ascertained. This new understanding will lend itself not only to understanding the biological function of the cell membrane but also to studying new biomimetic systems such as sensors and targeted drug delivery.

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6.0 CONCEPT OPTIMIZATION (INCLUDING R&D) IMPORTANT TO OPTIMIZE PERFORMANCE, RELIABILITY, AND COST

6.1 ACCELERATOR SYSTEMS

The second target station scenarios assume that the accelerator systems will ultimately be capable of 3 MW, which is at the upper range of the expected performance after the PUP. The PUP R&D plan includes ion source development, superconducting linac (SCL) improvements, and stripper foil development. All of these efforts are crucial for the success of the second target station.

In addition to the R&D issues identified by the PUP, the STS concept includes further development needs. In particular the increased beam loading associated with not chopping the beam for the long pulses going to the STS has a large impact on the linac, if unchopped beam currents greater than 43 mA are employed. These are largely engineering developments, but some additional concept optimization could help minimize the cost impacts, the time requirements for installing equipment upgrades, and the time needed to learn to operate the upgraded equipment reliably.

There are several outstanding issues associated with the choice of the long-pulse mode of beam delivery to the STS. Foremost is how much additional beam could be delivered in long-pulse vs short-pulse mode for an acceptable beam loss limit. Other issues related to the interleaving production of short and long pulses to the two targets include (1) design of an appropriate extraction system, (2) production of an appropriate beam distribution on the STS in long-pulse mode, and 3) control/timing system modifications. Many of these issues have been proposed for investigation in an internal Laboratory Directed Research and Development project.

6.2 TARGET STATION

6.2.1 Neutronics

Optimization studies of the STS have indicated that significant gains of long-wavelength neutrons can be realized by using large para-hydrogen moderators. The importance of para-hydrogen cannot be overstated, as the large cross section of ortho-hydrogen results in a poorly performing moderator system in this geometry. Development work on the understanding of ortho/para-hydrogen kinetics of irradiated hydrogen will be important to understanding the need for a catalyst, sizing the catalyst, and understanding the per-pulse generation of ortho-hydrogen due to irradiation, which cannot be impacted with a catalyst.

The STS reference concept target system geometry has been based upon moderator, premoderator, and reflector materials that have proved reliable in existing target systems. Advanced materials, particularly for premoderators and reflectors, have potential to improve the system performance or significantly reduce the cost while maintaining performance. To computationally evaluate additional premoderator and reflector materials, such as mesitylene, titanium hydride, and so on, requires the creation of scattering kernels at the proper temperature for these materials. In addition to the creation of these scattering kernels, verification of the kernel accuracy based upon neutron scattering or moderator measurement data will be an important part of the process.

6.2.2 Target Assemblies

Cavitation damage to the target mercury vessel is expected to be much less severe or possibly not a problem for long-pulse operation. Confirmation of this expectation, however, is planned as an R&D activity. Cavitation in the mercury is known to occur for short-pulse operation (< 1 μsec pulses) because the heating rate is much greater than the thermal relaxation rate, and the resulting initial compression waves produce rarefaction waves after reflecting from the interface on the vessel shell. When the pulse length is approximately 1 msec, it is likely that relaxation can occur, reducing the initial level of compression; but since the mercury has been shown to cavitate at low negative pressures (1 to 2 atmospheres), an analysis of the pressure response is planned. This analysis will be based on the technique developed for the FTS mercury target pressure wave propagation, but modification of the simulation code is needed to simultaneously include long-pulse and cavitation effects. A range of long-pulse cases (power, beam pulse length) will be simulated and the propensity for cavitation evaluated. Confirmatory in-beam testing would also be done, most likely at the Los Alamos accelerator. This testing would be similar to the testing done there previously for SNS, but with long pulse-operation.

A rotating solid target design has the potential to provide a simple, robust, highly flexible, and long-lifetime alternative target for the SNS second target station that is insensitive to the selection of either long-pulse (~1 ms) or short-pulse (~1 μs) operation. Slow rotation (a few Hz) would greatly reduce the average power density and radiation damage. As a result, the cooling requirements would be relaxed, resulting in longer target lifetimes (years) and increased neutron production. Efficient coupling to the moderators can be achieved using smaller beam spot sizes. The principal issues are developing the mechanical design concepts, including target cooling; handling methods for the target, moderators, and reflectors; and optimizing the source geometry to fit the desired suite of neutron instruments. This option will be evaluated as part of the R&D program.

The large coupled moderators are responsible for most of the neutronic gain expected at the STS. Optimizing the thermal hydraulic and structural design of these moderators to maximize neutronic performance while minimizing structure to reduce heat loads will be a challenge. The largest comparable moderator design is at the J-PARC facility with a 140 mm internal diameter moderator designed for 1 MW operation. The STS design for 220 mm internal diameter and operation at 2 to 3 MW will require innovative structural and thermal-hydraulic design development. The R&D program will include mechanical design development, computational fluid dynamics design development for the hydrogen flow and heat removal within the moderators, and mock-up testing with a surrogate fluid to visualize the internal flow patterns for an optimized design.

6.3 INSTRUMENTS

As shown in Sect. 3.5, current technology would enable the construction of a suite of world-class instruments at the STS that would be much better than any currently available. However, by the time the STS is built, the technology for neutron scattering instruments and components is certain to have advanced; and it is prudent to carry out R&D to ensure that the instruments ultimately built at the STS can take full advantage of techniques and components that are state-of-the-art at that time. Such an R&D program would focus both on developing new techniques for neutron scattering measurements and on developing new or improved components for neutron scattering instrumentation.

6.3.1 New Measurement Techniques

A number of the instruments proposed for the STS make use of RRM or wavelength multiplication. These techniques have been successfully tested and extensively simulated, so there is little technical risk. However, further development of these techniques will be useful to ensure full optimization of the STS instruments.

Several other promising new measurement techniques have been proposed and carried to the point of proof-of-principle experiments. However, all of these techniques will require considerable development before they can lead to neutron scattering instruments at the STS.

TISANE [6.1] is a technique in which the beam is chopped at a high frequency while the sample is “pumped” by an external field and the detector is gated at yet another frequency. This technique can be used to probe relaxation times as short as a few μs, a time range that is not readily accessible to other neutron scattering techniques. However, this technique is still in the early stages of development, and there is still room for considerable improvement.

SERGIS [6.2] is a technique in which scattering angles of a broadly divergent beam are coded by the Larmor precession of neutron spins in a magnetic field in a variant of the well-known NSE method. SERGIS measures spatial correlations directly in real space rather than in reciprocal space and, in particular, measures lateral structural correlations in thin films, on surfaces, or at interfaces. Preliminary measurements with prototypes show the technique to be highly promising, with the potential to revolutionize the use of neutrons for probing lateral structures at surfaces. However, considerable development will be required before an STS instrument can be based on this technique.

MIEZE (modulation of intensity with zero effort) [6.3] is based on the NRSE technique but with all coils and the analyzer installed upstream from the sample. The resulting sinusoidal signal has the same frequency for all neutron wavelengths; but it can have the same phase at only one point, the so called spin echo point, which is downstream from the sample. The detector is installed very close to this point and must have very good timing characteristics. MIEZE is especially suited for measurements on protonated samples because polarization analysis is done upstream of the sample; therefore, the strong spin flip probability of hydrogen does not deteriorate the signal, in contrast to NSE or NRSE. This will be a particularly strong advantage for the study of dynamics in biological samples, if this technique can be developed to serve as the basis for one or more of the STS instruments.

Longitudinal NRSE [6.4] is a new implementation of the NRSE technique, in this case with longitudinal magnetic fields rather than the usual transverse fields. In this field geometry, the effect of beam divergence can be corrected by means of standard Fresnel coils while the other advantages of the NRSE technique over conventional NSE are maintained. It should therefore be possible for longitudinal NRSE to be extended to higher resolutions, enabling the study of even slower dynamical motions with correlations over longer time scales. As with the other techniques discussed, however, considerable development will be required before this technique can be routinely used for neutron scattering instruments.

6.3.2 Improved Instrument Components

Although the development of a totally new measurement concept can open up totally new areas to exploration, most of the major advancements in neutron scattering instrumentation have come about by improvements in the performance of instrument components. Steady incremental advances in components can lead to such large improvements in the measurement capabilities of instruments based on existing concepts that they enable qualitatively new science as well.

An area of component development that is still in its infancy is the use of neutron focusing devices to provide the very high intensity necessary for the study of smaller samples, and further development of such devices will be important for fully realizing the potential of many neutron scattering instruments at the STS. Another, similar development that has not yet reached wide application is focusing in the time domain, which can enable higher intensities by opening up the acceptances of various components while preserving and optimizing resolution.

Modern neutron sources and instrumentation are already pushing the rate and resolution limits of the detectors currently available, and this problem will be much more pronounced with the high fluxes available at the STS. R&D to increase the instantaneous data rate capabilities and/or the spatial resolution of the detectors will be critical for realizing the full capabilities of many of the STS instruments.

Many of the new instrument concepts to be explored for use at the STS instruments will depend on the manipulation of neutron spins (e.g., for spin-dependent measurement techniques such as spin-echo and for the study of magnetic scattering), so R&D aimed at developing better polarizers, analyzers, resonance coils, flippers, and so on will be very important.

The use of small samples and the design of the instruments for the concurrent use of many different measurement techniques mean that it will be necessary to develop new approaches to the sample environments. The small sample sizes will also open up the opportunity for measurements under extreme sample environment conditions, and appropriate sample environments will need to be developed.

Finally, modern instruments are becoming capable of collecting far larger quantities of data across much larger ranges of energy- and momentum-transfer space than were previously accessed. Currently existing analysis software is capable of extracting and analyzing only a limited portion of the information content from such large data sets, and it frequently requires many iterations before even that limited portion of the data can be adequately analyzed. Thus large gains in scientific capability can also arise from significant improvements in analysis software capability. The next generation of instrumentation to be developed for the STS will extend this trend, making it even more important to expend adequate resources on the development of analysis techniques and associated software.

6.3.3 Development Beamline(s)

Most of these development efforts cannot be fully evaluated and refined without significant access time for testing in a neutron beam. Therefore, central to a successful instrumentation R&D program will be adequate access to one or more test beams at the FTS, HFIR, or at other facilities, and later at the STS.

6.4 CONVENTIONAL FACILITIES

Figure 6.1 shows two potential alternative sites that could be used if there is an overriding reason that the proton beam for the STS should not go through the existing accumulator ring. Either of these sites would require significant site work and would require further evaluation to confirm its viability.

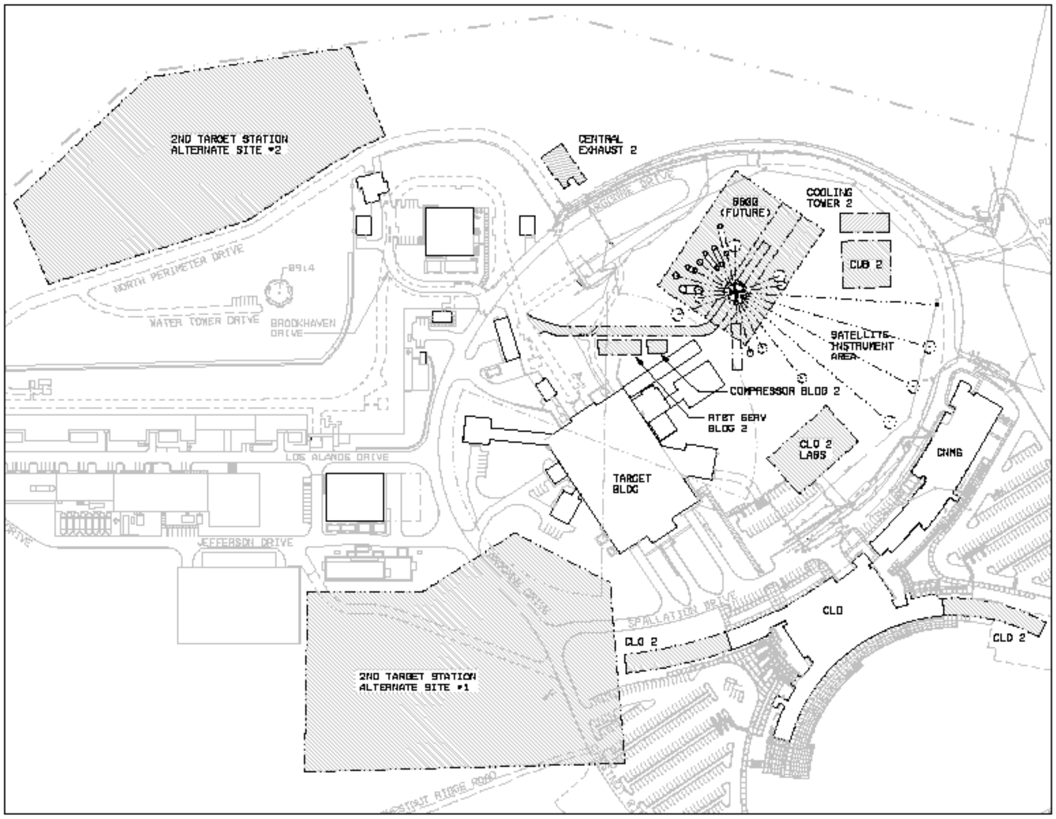

Fig. 6.1. Alternative reference concept layout of the STS. Two alternative sites are identified (hatched) for the STS facilities.

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7.0 OPPORTUNITIES FOR OPTIMIZATION OF INTERFACES WITH OPERATING SNS FACILITY

7.1 INTEGRATION/COORDINATION WITH PUP

There are opportunities for integration of efforts between the PUP and STS projects for issues related to the accelerator. Both projects require upgrades to the RF systems, but the different parameter choices outlined in Table 3.1 would involve different RF upgrade paths. The PUP upgrades are not compatible with the new STS requirements in that they do not consider increased beam loading resulting from the unchopped long-pulse-mode pulses for the STS in the case of unchopped beam current >43 mA. Folding in the STS requirements for the HVCM and RF upgrades would increase the costs presently being considered for the PUP but would be less costly and impose less schedule impact than reworking the entire HVCM and RF systems yet again for the STS.

The long-pulse mode of operation for the STS adds new ring extraction requirements. The planned PUP extraction upgrade may be modified if long-pulse mode is included. Ideally, the extraction region upgrades for accommodating higher energy and alternating short and long pulses should be considered together.

Some construction activities for both PUP and the STS will result in significant accelerator downtime. There is an opportunity to coordinate these activities to minimize the total downtime required at SNS. One such activity, tie-in of the proton beamline and associated underground tunnel to the second target station, could be accomplished during any long accelerator shutdown required for PUP to minimize the shutdown period required for the second target station.

7.2 INTEGRATION/COORDINATION WITH OTHER SNS SITE INFRASTRUCTURE IMPROVEMENTS

A number of new facilities have been funded or are being proposed for the Chestnut Ridge campus. It is desirable to consider the infrastructure needs of all the planned facilities to maximize the flexibility and potential uses of the site. For example, the cooling water needs for the entire site should be addressed in a unified way, as separate, standalone utilities would consume excessive real estate and probably would result in higher operating and maintenance costs. One option is to design utility systems to facilitate modular expansion to meet future needs.

The geographical layout of the Chestnut Ridge campus is such that a limited amount of land is available that can easily be developed for either planned or unanticipated needs. To maximize the potential for future expansions, it is critical that the planning process consider optimizing the available areas for development and integrating central utility systems.

The master site plan for Chestnut Ridge could be updated to reflect the latest siting decisions and planned new facilities.

7.3 INSTRUMENT SELECTION

If the time scale on which the STS is to be constructed were known, it could be considered in the planning for and selection of new instruments for both the FTS and HFIR. Such an integrated strategy would optimize the use of the SNS and HFIR resources for overall scientific performance.